Dynamics and Statistical Physics Division
Fachverband Dynamik und Statistische Physik (DY)

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Overview of Invited Talks and Sessions

(Lecture rooms: HÜL 186, ZEU 118, ZEU 146, and ZEU 160; Posters: P1 and P3)

Invited Talks

DY 2.1	Mon	9:30–10:00	HÜL 186	**Welcome to Twin Peaks: momentum-space signatures of Anderson localization** — •Cord A. Müller
DY 5.1	Mon	15:00–15:30	HÜL 186	**Feedback and information processing in stochastic thermodynamics** — •Udo Seifert
DY 5.2	Mon	15:30–16:00	HÜL 186	**Thermophoretic trapping and steering of single nano-objects with plasmonic nanostructures** — •Frank Cichos, Andreas Bregulla, Marco Braun, Haw Yang
DY 5.7	Mon	17:15–17:45	HÜL 186	**Feedback control in quantum transport** — •Clive Emary
DY 6.1	Mon	15:00–15:30	ZEU 160	**Odd Bose condensation far from equilibrium** — Daniel Vorberg, Waltraut Wustmann, Roland Ketzmerick, •André Eckardt
DY 8.7	Mon	16:45–17:15	ZEU 118	**Self-organized criticality in Hamiltonian spin systems: intriguingly ordinary or ordinarily intriguing?** — •Helmut G. Katzgraber
DY 9.1	Tue	9:30–10:00	HÜL 186	**From epilepsy to migraine to stroke: A unifying framework.** — •Markus A Dahlem
DY 9.2	Tue	10:00–10:30	HÜL 186	**Non-standard Interactions in Networks: Synchrony and the Emergence of Neural Activity Patterns** — •Marc Timme, Sven Jahnke, Raoul-Martin Memmesheimer, Wen-Chuang Chou, Christian Tetzlaff
DY 9.3	Tue	10:30–11:00	HÜL 186	**Towards a dynamic map of neuronal circuits** — •Alipasha Vaziri
DY 21.10	Wed	17:30–18:00	HÜL 186	**Episodic Precipitation** — •Jürgen Vollmer
DY 26.1	Thu	9:30–10:00	HÜL 186	**The memory of sand** — •Matthieu Wyart
DY 26.2	Thu	10:00–10:30	HÜL 186	**Complex rheology at the jamming transition: shear thickening, shear thinning, shear banding** — •Claus Heussinger
DY 43.1	Fri	9:30–10:00	HÜL 186	**Critical Rheology of Weakly Vibrated Granular Media** — •Martin Van Hecke
DY 43.5	Fri	11:00–11:30	HÜL 186	**A Granular Ratchet: Spontaneous Symmetry Breaking and Fluctuation Theorems in a Granular Gas** — •Devaraj van der Meer, Sylvain Joubaud, Peter Eshuis, Ko van der Weele, Detlef Lohse

Invited talks of the joint symposium SYEE

See SYEE for the full program of the symposium.

SYEE 1.1	Wed	15:00–15:30	HSZ 02	**Smart Grids - From incentives to coupled markets** — •Rudolf Sollacher
SYEE 1.2	Wed	15:30–16:00	HSZ 02	**Energy and the economy** — •Reiner Kümmel
SYEE 1.3	Wed	16:00–16:30	HSZ 02	**Planetary constraints to energy supply and the economy** — •Oliver Richters
SYEE 1.4	Wed	16:45–17:15	HSZ 02	**Identifying critical infrastructures in complex supply networks** — •Dirk Witthaut
SYEE 1.5	Wed	17:15–17:45	HSZ 02	**Short time fluctuations of renewable energies** — •Joachim Peinke, M. Reza Rahimi Tabar, Patrick Milan, Matthias Wächter

Invited talks of the joint symposium SYCP

See SYCP for the full program of the symposium.

SYCP 1.1	Thu	9:30–10:00	HSZ 02	**Why do polymer collapse and polymer topology frustrate each other** — •Alexander Y. Grosberg
SYCP 1.2	Thu	10:00–10:30	HSZ 02	**Nanoscopy of nuclear Genome Structure** — •Christoph Cremer
SYCP 1.3	Thu	10:30–11:00	HSZ 02	**Blood Clotting Inspired Polymer Physics** — •Alfredo Alexander-Katz
SYCP 1.4	Thu	11:15–11:45	HSZ 02	**Modeling dynamic spatial genome organization in yeast** — •Christophe Zimmer
SYCP 1.5	Thu	11:45–12:15	HSZ 02	**Ring polymers in the melt state: the physics of crumpling** — •Ralf Everaers, Angelo Rosa

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Sessions

DY 1.1–1.3	Sun	16:00–18:15	HSZ 105	**Tutorial: Non-Equilibrium Dynamics**
DY 2.1–2.8	Mon	9:30–12:00	HÜL 186	**Quantum Dynamics, Decoherence and Quantum Information**
DY 3.1–3.8	Mon	9:30–11:45	ZEU 160	**Statistical Physics far from Thermal Equilibrium - Part I**
DY 4.1–4.7	Mon	9:30–11:15	ZEU 146	**Anomalous Diffusion**
DY 5.1–5.7	Mon	15:00–17:45	HÜL 186	**Focus Session: Feedback Control of Nonlinear Soft and Hard Matter Systems (joint session DY/CPP)**
DY 6.1–6.8	Mon	15:00–17:30	ZEU 160	**Statistical Physics far from Thermal Equilibrium - Part II**
DY 7.1–7.9	Mon	15:00–17:30	ZEU 146	**Glasses (joint session DY/ DF/ CPP)**
DY 8.1–8.11	Mon	15:00–18:15	ZEU 118	**Critical Phenomena and Phase Transitions**
DY 9.1–9.5	Tue	9:30–11:30	HÜL 186	**Focus Session: Dynamical Patterns in Neural Systems: From Brain Function to Dysfunction (joint session DY/ BP)**
DY 10.1–10.11	Tue	9:30–12:30	ZEU 160	**Nonlinear Stochastic Systems**
DY 11.1–11.11	Tue	9:30–12:30	ZEU 146	**Microswimmers (joint session DY/ BP)**
DY 12.1–12.7	Tue	9:30–11:30	ZEU 118	**Complex Fluids and Soft Matter (joint session DY/ CPP/ BP)**
DY 13.1–13.38	Tue	9:30–12:30	P1	**Poster - Glasses / Stat. Phys. Bio. / Networks (joint session DY/BP/CPP/SOE)**
DY 14.1–14.4	Tue	15:00–16:00	GÖR 226	**Networks, From Topology to Dynamics I (joint session SOE/DY/ BP)**
DY 15.1–15.8	Wed	9:30–11:45	HÜL 186	**Nonlinear Dynamics, Synchronization and Chaos - Part I**
DY 16.1–16.9	Wed	9:30–12:00	ZEU 160	**Statistical Physics in Biological Systems (joint session DY/ BP)**
DY 17.1–17.8	Wed	9:30–11:45	ZEU 146	**Modeling and Data Analysis**
DY 18.1–18.12	Wed	9:30–12:45	ZEU 118	**Granular Matter / Contact Dynamics**
DY 19.1–19.6	Wed	11:45–13:15	GÖR 226	**Energy Meets Economy: Dynamics and Statistics of Future Energy Systems (joint session SOE/DY/ jDPG)**
DY 20.1–20.8	Wed	14:00–16:30	ZEU 250	**Focus Session: Modelling of Non-linear Dynamics in Biological Movement (joint session BP/ DY)**
DY 21.1–21.10	Wed	15:00–18:00	HÜL 186	**Pattern Formation**
DY 22.1–22.12	Wed	15:00–18:15	ZEU 160	**Statistical Physics (general)**
DY 23.1–23.14	Wed	15:00–18:45	ZEU 146	**Quantum Chaos**

DY 24.1–24.14	Wed	15:00–18:45	ZEU 118	**Networks - Statistics and Dynamics (joint session DY/ BP/ SOE)**
DY 25.1–25.5	Wed	15:00–17:45	HSZ 02	**Symposium SYEE: Energy Meets Economy: Dynamics and Statistics of Future Energy Systems (joint session SOE/ DY)**
DY 26.1–26.9	Thu	9:30–12:30	HÜL 186	**Focus Session: Slow Dynamics in Glasses and Granular Matter I (joint session DY/ CPP/ DF)**
DY 27.1–27.9	Thu	9:30–12:00	ZEU 160	**Nonlinear Dynamics, Synchronization and Chaos - Part II**
DY 28.1–28.10	Thu	9:30–12:15	ZEU 146	**Extreme Events**
DY 29.1–29.5	Thu	9:30–12:15	HSZ 02	**Symposium SYCP: The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (joint session CPP, BP,DY)**
DY 30.1–30.9	Thu	10:00–12:30	POT 081	**Graphene-Like Materials: Silicene, MoS_2 and Relatives (joint session HL/DY/DS/MA/O/TT)**
DY 31.1–31.5	Thu	11:00–12:15	GÖR 226	**Evolutionary Game Theory and Economic Models (joint session SOE/ BP/ DY)**
DY 32.1–32.3	Thu	11:45–12:45	ZEU 114	**Glasses and Glass Transition - Part I (joint session CPP/ DY/DF)**
DY 33.1–33.3	Thu	12:15–13:00	GÖR 226	**Networks, From Topology to Dynamics - Part II (joint session SOE/ DY/ BP)**
DY 34.1–34.5	Thu	15:00–17:45	HSZ 02	**Symposium SYGP: Stochastic Dynamics of Growth Processes in Biological and Social Systems**
DY 35.1–35.9	Thu	15:00–17:30	HÜL 186	**Reaction-Diffusion Systems**
DY 36.1–36.8	Thu	15:00–17:15	ZEU 160	**Brownian Motion and Transport**
DY 37.1–37.6	Thu	15:00–16:30	ZEU 146	**Fluid Dynamics and Turbulence**
DY 38.1–38.7	Thu	15:00–17:30	ZEU 114	**Glasses and Glass Transition - Part II (joint session CPP/ DY/DF)**
DY 39.1–39.11	Thu	15:00–18:00	POT 081	**Graphene: Spintronics, Transistors, and Sensors (joint session HL/DY/DS/MA/O/TT)**
DY 40.1–40.33	Thu	17:00–19:00	P3	**Poster - Quantum Systems/ Stat. Phys./ Diffusive Process**
DY 41.1–41.48	Thu	17:00–19:00	P3	**Poster - Pattern/ Nonlinear Dyn./ Fluids/ Granular/ Critical Phen.**
DY 42	Thu	19:00–20:00	ZEU 160	**Annual General Meeting of DY**
DY 43.1–43.8	Fri	9:30–12:15	HÜL 186	**Focus session: Slow Dynamics in Glasses and Granular Matter II (joint session DY/ CPP/ DF)**
DY 44.1–44.7	Fri	11:15–13:00	POT 081	**Graphene: Interaction With the Substrate (joint session HL/DY/DS/MA/O/TT)**
DY 45.1–45.7	Fri	11:30–13:15	CHE 89	**Graphene (joint session DS/ TT/ MA/ HL/ DY/ O)**

Annual General Meeting of the Dynamics and Statistical Physics Division

Thursday 19:00–20:00 ZEU 160

All members of the Dynamics and Statistical Physics Division are invited to participate in our annual meeting. The proposed topics are:

- reports and comments on the actual meeting
- spring meeting 15.03. - 20.03.2015 in Berlin
- miscellaneous

DY 1: Tutorial: Non-Equilibrium Dynamics

Classical thermodynamics deals with systems in (quasi) equilibrium. However, due to external energy supply or removal a system can be driven out of equilibrium. As a consequence the behavior of these systems differs in several respects from those in classical thermodynamics.

This tutorial is intended to give especially young scientists the opportunity to learn more about the subject of non-equilibrium processes. Besides the introduction to some fundamental concepts several example systems will be discussed.

Time: Sunday 16:00–18:15 Location: HSZ 105

Tutorial DY 1.1 Sun 16:00 HSZ 105

Nonlinear deterministic and nonlinear stochastic processes as models in non-equilibrium physics — •Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Due to friction, every macroscopic system eventually enters a rest state unless it is externally driven. Whereas purely constant or periodic driving leads us to deterministic models, additional coupling to a heat bath results in non-equilibrium stochastic processes. This tutorial, to be understood in conjunction with the two other talks given by H. Stark and U. Seiffert, tries to cover the most relevant and most striking aspects of low-dimensional deterministic and stochastic dynamics of driven systems: bifurcations, lack of a superposition principle, self-organisation, and the interpretation as an entropy producing/exporting system.

Tutorial DY 1.2 Sun 16:45 HSZ 105

Stochastic Thermodynamics — •Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Germany

In this talk, I will give an introduction to the emerging field of stochastic thermodynamics and illustrate its main concepts with recent experimental data. Stochastic thermodynamics provides a framework for describing small systems embedded in a heat bath and externally driven to non-equilibrium [1]. Examples are colloidal particles in time-dependent optical traps, single biomolecules manipulated by optical tweezers or AFM tips, and motor proteins driven by ATP excess. The notions of classical thermodynamics like applied work, exchanged heat and total entropy production valid there on the ensemble level can now be consistently identified and measured on the level of an individual stochastic trajectory. Moreover, exact results that refine the second law like the Jarzynski relation and fluctuation theorems for entropy production can be proven. Using these concepts, the efficiency of nanoscopic machines like molecular motors can be determined and their performance be optimized.

[1] U. Seifert, Rep. Prog. Phys. 75, 126001, 2012.

Tutorial DY 1.3 Sun 17:30 HSZ 105

Active motion at low Reynolds number — •Holger Stark — Institut für Theoretische Physik, TU Berlin, D-10623 Berlin, Germany

Starlings over Rome form dynamic swarms, fishes in water move collectively in fish schools. Zooming from the macroscopic into the microscopic world, bacteria also show intricate collective behavior.

However, on the micron scale swimming in aqueous environment requires different strategies than in the macroscopic world since at low Reynolds number drifting by inertia is not possible. Biological swimmers like bacteria and artificial microswimmers constantly consume energy to move forward. They are always in nonequilibrium.

The talk demonstrates some swimming strategies from nature but also of man-made microswimmers. It then illustrates at a few examples, how active motion reveals itself already on the single-swimmer level but also in the collective properties when many swimmers interact.

DY 2: Quantum Dynamics, Decoherence and Quantum Information

Time: Monday 9:30–12:00 Location: HÜL 186

Invited Talk DY 2.1 Mon 9:30 HÜL 186

Welcome to Twin Peaks: momentum-space signatures of Anderson localization — •Cord A. Müller — Fachbereich Physik, Universität Konstanz

Quantum Systems with structural disorder present unusual challenges when is comes to understanding long-time limits of their phase-space dynamics. In particular, Anderson localization is well known to suppress classical diffusion of (matter) waves in real space—but much less is known about its momentum-space signatures.

Recently, a new signature of strong Anderson localization has been discovered for ultracold atoms following a quantum quench: a twin-peak signal in the particles' momentum distribution. This structure combines the familiar back-scattering peak with a coherent forward-scattering peak [1]. The forward peak appears to be a genuine signal for the onset of strong localization, surviving in the presence of weak magnetic fields. Recent non-perturbative calculations in a quasi-1D setting [2] have confirmed that the forward peak can serve as a reliable signature of Anderson localization. This theory describes the peak's temporal genesis as well as its aymptotic features such as width and height, and arguably presents the only instance where the temporal evolution of a strong localization phenomenon can be described analytically at all times.

[1] T. Karpiuk et al., PRL 109, 190601 (2012)
[2] T. Micklitz et al., arXiv:1311.2268

DY 2.2 Mon 10:00 HÜL 186

Adiabatic-Markovian Dynamics at Avoided Crossings — •Peter Nalbach — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstr. 9, 20355 Hamburg

In order to study Landau-Zener transitions at avoided crossings under the influence of environmental fluctuations we derive effective nonequilibrium Bloch equations. Thereby, we employ an adiabatic-Markovian approximation which results in effectively time-dependent relaxation and dephasing rates and a time-dependent quasi-equilibrium statistical operator to which the system is driven. At weak coupling, where in a static case a Markovian approximation is valid, we observe very good agreement for the full driving speed range between the nonequilibrium Bloch equations predictions and numerical exact data for the Landau-Zener transition and the excitation survival probability [1]. The nonequilibrium Bloch equations, thus, allow for an efficient tool to analyze and model the dynamics in driven double quantum dot [2] and other qubit realizations.

[1] P. Nalbach and M. Thorwart, Phys. Rev. Lett. 103, 220401 (2009) & Chem. Phys. 375, 234 (2010).

[2] P. Nalbach, J. Knörzer and S. Ludwig, Phys. Rev. B 87, 165425 (2013).

DY 2.3 Mon 10:15 HÜL 186

A generalized quantum regression theorem for non-Markovian two-time correlation functions of system operators — •Jinshuang Jin[1,2,3], Michael Marthaler[3,4], and Gerd Schön[3,4] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Karlsruhe, Germany — [2]Department of Physics, Hangzhou Normal University, Hangzhou, China — [3]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology(KIT), Karlsruhe, Germany — [4]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology, Karlsruhe, Germany

We present an efficient scheme for the calculation of two-time correlation functions for open quantum systems with memory effect. This

scheme is the generalization of the quantum regression theorem with the consideration of non-Markovian effects. We further apply the present method to both Ferminonic and Bosonic systems. The former is to study the charge fluctuation spectrum of the interacting quantum dots in the sequential tunneling regime. The latter is to investigate the non-Markovian effect of the phonon bath on the emission spectrum of a cavity. The characteristic non-Markovian features in the spectra are explored.

DY 2.4 Mon 10:30 HÜL 186

Coherence phase diagram and a quench dynamics of a spin-boson model. — •Oleksiy Kashuba[1], D.M. Kennes[2], M. Pletyukhov[2], V. Meden[2], and H. Schoeller[2] — [1]Institut für Theoretischen Physik, Technische Universität Dresden — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen

We study the non-Markovian dynamics of the small dissipative quantum system coupled to an thermodynamically equilibrated environment. The memory effects probed by the quenching of the coupling strength. We discovered the contra-intuinive tendency of the system to the enhancement of the coherence in response to stronger memory of the incoherent behaviour before the quench. Studying the dynamics of the system at different coupling and temperatures we revealed several distinct "phases" by discriminating between the dynamics on intermediate and long time scales. Surprisingly, elevated temperature can render the system "more coherent" by inducing a transition from the partially coherent to the coherent regime.

15 min break

DY 2.5 Mon 11:00 HÜL 186

Beyond Born-Markov: validity, dependencies and the initial state problem — •Christian Karlewski, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, KIT, 76128 Karlsruhe

We expand the master equation for an open quantum system in terms of the Born and the Markov approximation. This makes it possible to calculate higher order-terms in the coupling strength to the bath beyond the famous Born-Markov approximation. Additionally, we are able to compare and distinguish between the terms belonging to Born or Markov approximation. The first issue we address with this approach is the initial state problem. Our method allows to quantify initial correlations and thus the error made by neglecting them. Secondly, we investigate the behaviour of a specific system, the spin boson model with an Ohmic noise with Drude-Lorentz cutoff, and we compare our computations with the Born-Markov approximation.

DY 2.6 Mon 11:15 HÜL 186

Dissipative dynamics and energy transfer of a harmonic oscillator coupled to nonthermal baths — •Daniel Pagel[1], Andreas Alvermann[1], Holger Fehske[1], Peter Nalbach[2], and Michael Thorwart[2] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald — [2]I. Institut für Theoretische Physik, Universität Hamburg

The dissipative dynamics of a quantum-mechanical system can be studied in a microscopic setting if one includes an explicit coupling to one or more baths of harmonic oscillators. Allowing for general nonequilibrium bath preparations instead of the usually employed thermal ones, we look at the long-time behavior of the dissipative harmonic oscillator coupled to one bath and prove that it equilibrates in the absence of isolated modes. The stationary density matrix in the long-time limit then depends on the initial bath state only. We discuss the requirements for full thermalization of the central oscillator. In the case of multiple baths, where stationary nonequilibrium states of the central oscillator become possible, we show that the fluctuations of the central oscillator follow an exact generalized nonequilibrium fluctuation relation. Finally, we discuss the generalization of the cumulant generating function for the energy transfer through the oscillator to the nonthermal situation.

DY 2.7 Mon 11:30 HÜL 186

Optimal control of non-interacting (quantum) harmonic oscillators and qubits — •Frank Boldt and Karl Heinz Hoffmann — Professur Theoretische Physik, insbesondere Computerphysik, Technische Universität Chemnitz

In this talk the time-optimal and decoherence free control of an ensemble of non-interacting (quantum) harmonic oscillators is given, using an geometrical approach based on the Casimir companion [1]. These time-optimal decoherence free passages are shortcuts to adiabaticity. Therefore fast optimal cooling processes are possible and maximum cooling rates will be given [2]. Further, time-optimal and decoherence free controls of an ensemble of non-interacting qubits will be deduced as a second example [3].
The optimal controls presented are piece-wise continuous functions (Bang-Bang controls) and thus hard to realize experimentally. As an outline, bounds for continuous controls with finite switching times were calculated to give experimenters hard limits for instance to adjust their experimental realized version of the control by a feedback loop.

[1] F. Boldt et al., PRA 87, 022116 (2013)

[2] P. Salamon et al., Phys. Chem. Chem. Phys., 2009, 11, 1027-1032

[3] F. Boldt et al., EPL 99, 40002 (2012)

DY 2.8 Mon 11:45 HÜL 186

Dynamics of entanglement entropy and entanglement spectrum crossing a quantum phase transition — •Elena Canovi[1], Elisa Ercolessi[2], Piero Naldesi[2], Luca Taddia[2], and Davide Vodola[2,3] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Dipartimento di Fisica e Astronomia dell'Università di Bologna and INFN, Sezione di Bologna, Via Irnerio 46, 40127 Bologna, Italy — [3]PCMS (UMR 7504) and ISIS (UMR 7006), Université de Strasbourg and CNRS, Strasbourg, France

We study the time evolution of entanglement entropy and entanglement spectrum in a finite-size system which crosses a quantum phase transition at different speeds. We focus on the Ising model with a time-dependent magnetic field, which is linearly tuned on a time scale τ. The time evolution of the entanglement entropy displays different regimes depending on the value of τ, showing also oscillations which depend on the instantaneous energy spectrum. The entanglement spectrum is characterized by a rich dynamics where multiple crossings take place with a gap-dependent frequency. Moreover, we investigate the Kibble-Zurek scaling of entanglement entropy and Schmidt gap.

DY 3: Statistical Physics far from Thermal Equilibrium - Part I

Time: Monday 9:30–11:45 Location: ZEU 160

DY 3.1 Mon 9:30 ZEU 160

High-precision work distributions for extreme non-equilibrium processes in large systems — •Alexander K. Hartmann — Institut of Physics, University of Oldenburg, Germany

The distributions of work for strongly non-equilibrium processes are studied using a very general form of a large-deviation approach, which allows one to study distributions down to extremely small probabilities of almost arbitrary quantities of interest for equilibrium, non-equilibrium stationary and even non-stationary processes. The method is applied to varying quickly the external field in a wide range $B = 3 \leftrightarrow 0$ for critical ($T = 2.269$) two-dimensional Ising system of size $L \times L = 128 \times 128$. To obtain free energy differences from the work distributions, they must be studied in ranges where the probabilities are as small as 10^{-240}, which is not possible using direct simulation approaches. By comparison with the exact free energies, one sees that the present approach allows one to obtain the free energy with a very high relative precision of 10^{-4}. This works well also for non-zero field, i.e., for a case where standard umbrella-sampling methods seem to be not so efficient to calculate free energies. Furthermore, for the present case it is verified that the resulting distributions of work fulfill Crooks theorem with high precision. Finally, the free energy for the Ising magnet as a function of the field strength is obtained.

DY 3.2 Mon 9:45 ZEU 160

Unifying three perspectives on information processing in stochastic thermodynamics — •Andre C Barato and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart 70550

The relation between information and thermodynamics may be studied using three different approaches: (i) measurement and control, (ii) a tape interacting with a system or (iii) by identifying an implicit Maxwell demon in steady state transport. For a single paradigmatic model we derive the three corresponding second laws from one master fluctuation theorem and discuss their relationship. In particular, we show that both the entropy production involving mutual information between system and controller and the one involving a Shannon entropy difference of an information reservoir like a tape carry an extra term different from the usual current times affinity. Moreover, comparing the usual entropy production from stochastic thermodynamics with the one obtained in approach (ii), we show that the former includes the thermodynamic cost of resetting the tape. Finally, inspired by the discussion on the paradigmatic model we generalize stochastic thermodynamics to the presence of an information reservoir.

Reference: arXiv:1308.4598 (2013)

DY 3.3 Mon 10:00 ZEU 160

Bayesian prior-predictive value for multi-modal distributions: thermodynamic integration, or fast-growth? — •Alberto Favaro, Elena Barykina, Daniel Nickelsen, and Andreas Engel — Institut für Physik, Carl-von-Ossietzky Universität, 26111 Oldenburg, Germany

In Bayesian inference, the prior-predictive value allows one to select the model, among different candidates, that fits the data best [Lartillot and Philippe, Syst. Biol. 55, 195-207 (2006)]. A common difficulty, when analysing data through Bayesian methods, is the evaluation of high-dimensional integrals. Techniques that originated in statistical physics, such as thermodynamic integration and fast-growth methods, can be used to mitigate this problem.

Naively, if the distribution of data is multi-modal, one expects that fast-growth algorithms, inspired by the Jarzynski equation, outperform thermodynamic integration. In fact, this last technique does not reliably sample all modes, as it often gets trapped around a maximum. The results of Ahlers and Engel for a bimodal Gaussian distribution appear to confirm this [Eur. Phys. J. B62, 357-364 (2008)]. Nevertheless, the estimate of the prior-predictive value, as obtained from a Jarzynski-like equation, is severely biased. By means of a careful error analysis, we determine the conditions under which a given method is to be preferred. Moreover, it is observed that fast-growth simulations are particularly efficient when computing averages with respect to the posterior distribution.

DY 3.4 Mon 10:15 ZEU 160

Extensions to Endoreversible Modelling — •Katharina Wagner and Karl Heinz Hoffmann — Technische Universität Chemnitz

In endoreversible thermodynamics irreversible processes and systems are split into reversible subsystems and interactions in between them. The irreversibilities are completely described by the interactions between the reversible subsystems. Interactions consist of two fluxes, i. e. energy and an extensive quantity, and are characterized by transport laws.

The standard formalism [1] is extended to model mass fluxes with more than one extensive quantity as carrier for the energy, since the different extensive quantities are usually not independent and need to be treated together. Irreversible systems with gases, like pressure regulators or throttles, are presented to demonstrate endoreversible modelling and quantification of entropy production in the model.

[1] Hoffmann, K. H., Burzler, J. M. and Schubert, S., J. Non-Equilib. Thermodyn. Vol. 22, 1997, No. 4

DY 3.5 Mon 10:30 ZEU 160

Emerging Smectic Phases in Simple Active Particle Models — •Pawel Romanczuk[1], Sandrine Ngo[2], and Hugues Chate[3] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Dept. of Physics, IPAM and ICSMB, University of Aberdeen, United Kingdom — [3]CEA-Saclay, Service de Physique de l'Etat Condensé, CEA-Saclay, Giv-sur-Yvette, France

Recently, several theoretical predictions have been made on so-called active smectics based on hydrodynamic theories derived solemnly from symmetry arguments [1,2]. Here, we show how the mere addition of pairwise repulsive interaction to alignment-only, self-propelled particle models generically gives rise to active smectic phases, which we study numerically in two space dimensions. The versatility of our approach allows us to study polar as well as apolar smectics of various types (A, C, and a new smectic P phase where particles form files so that the orientational order of the particles is parallel to the smectic stripes). We find that smectic order is rather weak: it is quasi-long-range up to some model-dependent size, but quickly breaks down in larger systems due to the spontaneous nucleation of dislocations and the presence of a long-wavelength undulation instability. Furthermore, our study also reveals a number of unexpected collective dynamical properties such as spontaneous global rotation of both orientational and smectic order.

[1] Adhyapak, T. et al, Phys Rev Lett 110, 11, 118102 (2013)
[2] Chen, L. and Toner, J., Phys Rev Lett 111, 8, 088701 (2013)

15 min break

DY 3.6 Mon 11:00 ZEU 160

Non-monotonic Density in the Compressible Car Parking Problem — •Johannes Nuebler, Brendan Osberg, and Ulrich Gerland — Arnold-Sommerfeld Center for Theoretical Physics and Center for NanoScience, Theresienstraße 37, 80333 München

The non-equilibrium dynamics of the one-dimensional adsorption-desorption process, the so-called "car parking problem", have been extensively studied. For fast adsorption, starting from an empty line, the covered fraction quickly reaches a plateau at which point all "parking spots" are too short for further adsorption. Thereafter, equilibrium is approached through much slower collective rearrangements.

Motivated by histone proteins on DNA, we generalize the adsorption-desorption process to soft particles. In this "compressible car parking problem", the particle density increases much faster and can be non-monotonic. We attribute this to the history of the parking spot size distribution and study its non-equilibrium thermodynamics.

DY 3.7 Mon 11:15 ZEU 160

Uncovering wind turbine properties through two-dimensional stochastic modeling of wind dynamics — Frank Raischel[1], •Teresa Scholz[2,3], Vitor V. Lopes[4], and Pedro G. Lind[5] — [1]Instituto Dom Luiz, CGUL, 1749-016 University of Lisbon, Lisbon, Portugal — [2]Center for Theoretical and Computational Physics, University of Lisbon, Av. Prof. Gama Pinto 2, 1649-003 Lisbon, Portugal — [3]Departamento de Física, Faculdade de Ciências da Universidade de Lisboa, 1649-003 Lisboa, Portugal — [4]Energy Systems Modeling and Optimization Unit, National Laboratory for Energy and Geology (LNEG), Estrada do Paço do Lumiar 22, 1649-038 Lisbon, Portugal

— [5]ForWind and Institute of Physics, Carl-von-Ossietzky University of Oldenburg, DE-26111 Oldenburg, Germany

Using a method for stochastic data analysis, borrowed from statistical physics, we analyze synthetic data from a Markov chain model that reproduces measurements of wind speed and power production in a wind park in Portugal. We first show that our analysis retrieves indeed the power performance curve, which yields the relationship between wind speed and power production and we discuss how this procedure can be extended for extracting unknown functional relationships between pairs of physical variables in general. Second, we show how specific features, such as the rated speed of the wind turbine or the descriptive wind speed statistics, can be related with the equations describing the evolution of power production and wind speed at single wind turbines.

DY 3.8 Mon 11:30 ZEU 160

Noise-insensitive energy transmission with magnetic coupling — •Benedikt Sabass — Princeton University

Systems with a magnetic coupling display unusual transport properties since time-reversal symmetry is broken. I study energy transmission in coupled oscillators, as it could be realized, e.g., with electronic circuits. Remarkably, magnetic coupling can render energy transmission in certain networks insensitive to perturbations from the outside. The mechanism and conditions for this passive noise compensation are discussed. I conclude with the idea for an application.

DY 4: Anomalous Diffusion

Time: Monday 9:30–11:15 Location: ZEU 146

DY 4.1 Mon 9:30 ZEU 146

Lévy walks, random time averaged diffusivities and a no-go theorem for ergodicity and an Einstein Relation — •Daniela Froemberg — Max Planck Institute for the Physics of Complex Systems, Dresden

We investigate a Lévy walk alternating between two states characterized by velocities of opposite sign. The sojourn times in either state are drawn according to power law probability distribution functions (pdf). Two different regimes are considered: The first case where the sojourn time pdf lacks its mean, corresponds to a ballistic regime. In the second case the mean of the sojourn time pdf exists while the second moment does not, which results in enhanced diffusion. The correlation functions and the discrepancies between time averaged and ensemble averaged mean squared displacements are investigated. The ballistic case exhibits weak ergodicity breaking and the fluctuations of the shifted time averaged mean squared displacements are universal. In the enhanced diffusion regime, the fluctuations of the time averaged mean squared displacements vanish at large times, yet very slowly. Moreover, we consider an external bias and present a no-go theorem for the generalized Einstein relation and ergodicity in the sense of equal time and ensemble averages.

DY 4.2 Mon 9:45 ZEU 146

Predicting and triggering anomalous Movements in Molecular Diffusion — •Sarah Hallerberg[1] and Astrid S. de Wijn[2] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Department of Physics, Stockholm University, 106 91 Stockholm, Sweden

Diffusion can be strongly affected by the appearance of ballistic trajectories (jumps) as well as subdiffusive sticking trajectories (sticks). Using statistical inference techniques, we investigate the appearance of jumps and sticks in molecular-dynamics simulations of diffusion in a prototype system, a benzene molecule on a graphite substrate. We find that specific fluctuations in certain, but not all, internal degrees of freedom of the molecule can be linked to the occurrence of either jumps or sticks. Furthermore, we show that by changing the prevalence of these predictors with an outside influence, the diffusion of the molecule can be controlled. The approach presented in this proof of concept study is very generic, and can be applied to larger and more complex molecules. Additionally, the predictor variables can be chosen in a general way so as to be accessible in experiments.

DY 4.3 Mon 10:00 ZEU 146

Functional Representation and Response Behavior of Fractional Fokker-Planck Equations — •Stephan Eule — MPIDS, Göttingen

The functional representation of stochastic processes provides a powerful method to calculate average values of path dependent observables. Here, the functional representation of Continuous Time Random Walks (CTRWs) and Fractional Fokker-Planck Equations is presented. This formulation, which is based on an alternative formulation of CTRWs, is then used to tackle the delicate and open problem of calculating the response of a CTRW to an external time-dependent perturbation. For the fractional Ornstein-Uhlenbeck process, the response function is calculated explicitly. It is proven that the fluctuation-dissipation theorem holds when the process is perturbed away from equilibrium.

DY 4.4 Mon 10:15 ZEU 146

Normal and anomalous fluctuation relations for Gaussian stochastic dynamics — Aleksei V. Chechkin[1], Friedrich Lenz[2], and •Rainer Klages[2] — [1]Inst. f. Theor. Physics, NSC KIPT, Kharkov, Ukraine — [2]Queen Mary U. of London, School of Math. Sci., UK

We study Fluctuation Relations (FRs) for Gaussian stochastic systems exhibiting anomalous diffusion. For this purpose we use a Langevin approach: We first briefly review the concept of transient work FRs for simple Langevin dynamics generating normal diffusion [1]. We then consider two different types of additive, power law correlated Gaussian noise [2]: (1) internal noise with a fluctuation-dissipation relation of the second type (FDR2), and (2) external noise without FDR2. For internal noise we find that FDR2 leads to conventional (normal) forms of transient work FRs. For external noise we obtain various forms of violations of normal FRs, which we call anomalous FRs. We argue that our theory is important for understanding experimental results on fluctuations in systems with long-time correlations, such as glassy dynamics [1].

[1] R.Klages, A.V.Chechkin, P.Dieterich, *Anomalous fluctuation relations*, book chapter in: R.Klages, W.Just, C.Jarzynski (Eds.), *Nonequilibrium Statistical Physics of Small Systems*, Wiley-VCH, Weinheim (2013)

[2] A.V.Chechkin, F.Lenz, R.Klages, J.Stat.Mech. L11001 (2012)

DY 4.5 Mon 10:30 ZEU 146

Relative entropies and anomalous diffusion — •Janett Prehl[1], Frank Boldt[1], Christopher Essex[2], and Karl Heinz Hoffmann[1] — [1]Technische Universität Chemnitz, Institut of Physics, Chemnitz, Germany — [2]University of Western Ontario, Department of Applied Mathematics, London, Canada

The entropy production paradox for anomalous diffusion processes describes a phenomenon where one-parameter families of dynamical equations, falling between the diffusion and wave equations, have entropy production rates (Shannon, Tsallis or Renyi) that increase toward the wave equation limit unexpectedly [1]. Moreover, also surprisingly, the entropy does not order the bridging regime between diffusion and waves at all [1]. In this talk we will present that different to entropies and entropy production rates relative entropies, with an appropriately chosen reference distribution, will order the bridging regime [2]. Thus, they provide a physically sensible way of setting which process is "nearer" to pure diffusion than another, placing pure wave propagation, desirably, "furthest" from pure diffusion. Furthermore, we examine the time behavior of the relative entropies under the evolution dynamics of the underlying one-parameter family of dynamical equations based on space-fractional derivatives [3].

[1] K.H. Hoffmann et al., *J. Non-Equilib. Thermodyn.* **37**, 393 (2012)

[2] J. Prehl et al., *Entropy* **14**, 701 (2012)

[3] J. Prehl et al., *Entropy* **15**, 2989 (2013)

DY 4.6 Mon 10:45 ZEU 146

Normal vs. anomalous transport by molecular motors in living cells — •Igor Goychuk[1], Vasyl Kharchenko[2], and Ralf Metzler[1,3] — [1]Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany — [2]Institute of Applied

Physics, NAS Ukraine, 40030 Sumy, Ukraine — [3]Department of Physics, Tampere University of Technology, 33101 Tampere, Finland

Discovery of anomalously slow diffusion of submicron particles in living cells provokes a number of questions, in particular, on active transport of such subdiffusing nanoparticles by molecular motors. Can such transport be normal or it is also anomalously slow? Can the same motors in the same cells realize both normal and anomalous transport and under which conditions? We answer these intriguing questions [1] within a non-Markovian generalization of standard Markovian continuous diffusion model of molecular motors with two conformational states by taking into account slowly decaying memory effects caused by the viscoelasticity of cytosol. Here we follow to and develop further a general approach to anomalous Brownian motors [2] which is based on Generalized Langevin Equation and its Markovian embedding [3]. Supported by DFG, Grant GO 2052/1-2

[1] Goychuk, I., Kharchenko, V., Metzler, R. arXiv:1309.6724 [physics.bio-ph] (2013); [2] Goychuk, I. Chem. Phys. 375, 450 (2010); Goychuk, I., Kharchenko, V. Phys. Rev. E 85, 051131 (2012); Kharchenko, V. and Goychuk, I. New J. Phys., 14, 043042 (2012); Phys. Rev. E 87, 052119 (2013); [3] Goychuk, I. Adv. Chem. Phys. 150, 187 (2012); Phys. Rev. E 80, 046125 (2009).

DY 4.7 Mon 11:00 ZEU 146

Spin diffusion in a ^{129}Xe crystal on mesoscopic length scales — •Alexander Potzuweit, Hagen Allmrodt, Lars Kraft, Anuschka Schaffner, and Heinz Jänsch — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

Medical applications using hyperpolarized ^{129}Xe have attracted much attention over the past years. To improve production and storage of hyperpolarized xenon further, a deeper understanding of the relaxation and transport processes is necessary. We employ NMR to investigate relaxation and spin diffusion in Xe films on mesoscopic length scales (nm...μm). Inside the NMR-spectrometer the hyperpolarized ^{129}Xe is frozen onto a Cu single crystal. At the xenon/metal interface the xenon will depolarize, so the copper serves as a polarization drain attached to one side of the xenon crystal. Using a simple diffusion model we analyze the experimental results like the spin transport to this drain as a function of time. By diluting the NMR-active isotope ^{129}Xe in the NMR-inactive isotope ^{132}Xe it is even possible to fine tune the diffusion constant or to inhibit spin diffusion altogether.

DY 5: Focus Session: Feedback Control of Nonlinear Soft and Hard Matter Systems (joint session DY/CPP)

Feedback control methods, which are well established in the field of nonlinear sciences, have recently entered new areas such as pattern formation in non-equilibrium soft-matter systems, Brownian transport and quantum transport. The focus session provides a platform for the presentation and discussion of state-of-the-art results and for pointing out open problems in this emerging field. (Organizers S. Klapp and E. Schöll)

Time: Monday 15:00–17:45 Location: HÜL 186

Invited Talk DY 5.1 Mon 15:00 HÜL 186

Feedback and information processing in stochastic thermodynamics — •Udo Seifert — II. Inst. für Theoretische Physik, Universität Stuttgart

Stochastic thermodynamics provides a framework for describing feedback control of colloidal and molecular systems [1]. A crucial concept is the notion of optimal finite-time protocols that transform a given initial distribution to a given final one in finite time with minimal thermodynamic cost [2]. If additional information becomes available through a measurement of the state of the system, one can thus even extract work from a single heat bath [3]. Fluctuation theorems taking into account this concept of information lead to bounds on the efficiency of such Brownian information machines [4]. These feedback-based schemes will be compared to autonomous information processing as it occurs in cellular sensing [5].

[1] U Seifert, Rep. Prog. Phys. 75, 126001, 2012
[2] T Schmiedl and U Seifert, Phys. Rev. Lett. 98, 108301, 2007
[3] M Bauer, D Abreu, and U Seifert, J. Phys. A 45, 162001, 2012
[4] D Abreu and U Seifert, Phys. Rev. Lett. 108, 030601, 2012
[5] AC Barato, D Hartich, and US, Phys. Rev. E 87, 042104, 2013

Invited Talk DY 5.2 Mon 15:30 HÜL 186

Thermophoretic trapping and steering of single nano-objects with plasmonic nanostructures — •Frank Cichos[1], Andreas Bregulla[1], Marco Braun[1], and Haw Yang[2] — [1]Molecular Nanophotonics Group, Institute of Experimental Physics I, University Leipzig, 04103 Leipzig, GERMANY — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544-2020, USA

The manipulation of single micro- and nano-particles or even single molecules in solution requires to beat Brownian motion with a mechanism that drives objects into a well defined direction. Such a mechanism is provided by the thermophoretic drift of nano-objects in a temperature gradient as generated by optically heated plasmonic nanostructures. Since these tiny heat sources can be switched optically at high frequencies, they provide new means of feedback controlled optical manipulations. Here we report on two experiments controlling individual particles in solution by such a feedback mechanism. The first experiment employs a self-propelled thermophoretic swimmer that is steered in solution by a real-time feedback of the swimmer orientation and position. This type of feedback controlled actuation predicts an increased positional control with decreasing particle size. The second experiment involves the trapping of single colloids and molecules in feedback controlled dynamic temperature fields. While the actual thermophoretic drift is repelling the object from the heat source, the dynamic switching provides and effective potential well, which can be shaped by the feedback details. Both experiments provide huge perspectives for study of interactions in well defined clusters of nano-objects.

DY 5.3 Mon 16:00 HÜL 186

Manipulating rheology of colloidal particles at surfaces — •Tarlan A. Vezirov, Sascha Gerloff, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Colloidal particles under the combined influence of an external driving force and restricted geometry exhibit a wealth of non-linear phenomena, which are relevant in diverse fields such as directed particle transport, sorting mechanisms and friction phenomena at the nanoscale. We perform computer simulations of a confined bilayer system of charged colloidal particles interacting via a combined softsphere- and Yukawa-potential. The model parameters are adjusted according to ludox silica particles, which we have previously studied under equilibrium conditions [1]. As a framework for solving the equation of motion, we employ overdamped Brownian dynamics simulations. Switching on an external shear flow we find, a sequence of states characterised by pinning, shear-induced melting and reentrant ordering into a moving hexagonal state with synchronised oscillations of the particles [1]. By adding an additional feedback equation of motion we are able to stabilise specific properties such as the degree of hexagonal ordering or the shear stress. This opens the route for a deliberate control of friction properties.

[1] S. Grandner and S.H.L. Klapp, J. Chem. Phys. **129**, 244703 (2008).
[2] T. A. Vezirov and S. H. L. Klapp, Phys. Rev. E **88**, 5 (2013).

DY 5.4 Mon 16:15 HÜL 186

Optimal control of particle separation in inertial microfluidics — •Christopher Prohm and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

At intermediate Reynolds numbers, particles in a microfluidic channel assemble at fixed distances from the channel axis and bounding walls [1]. This Segré-Silberberg effect can be described in terms of an ef-

fective lift force acting on the particles. Devices utilizing inertial lift forces for the separation of bacteria and red blood cells have recently been demonstrated [2]. The separation is most efficient for large size differences since the inertial lift force scales with the third power of the particle radius.

Here, we investigate the motion of a colloidal particle in microfluidic channels using mesoscopic simulations [3]. We show how the geometry of the channel influences inertial focussing. We also demonstrate that manipulating the axial or angular velocity of the particle modifies the inertial lift force profile which permits control of the lateral particle position. Finally we apply the theory of optimal control to the problem of particle sorting in inertial microfluidics [4]. We design optimal force profiles that are able to steer particles to desired lateral positions and, most importantly, to separate particles of similar size in a very robust fashion.

[1] G. Segré and A. Silberberg, *Nature*, **189**, 209 (1961).
[2] A. J. Mach and D. Di Carlo, *Biotechnol. Bioeng.*, **107**, 302 (2010).
[3] C. Prohm, M. Gierlak, and H. Stark *EPJE*, **35**, 80 (2012).
[4] C. Prohm, F. Tröltzsch, and H. Stark *EPJE*, **36**, 118 (2013).

15 min. break

DY 5.5 Mon 16:45 HÜL 186

Time-delayed feedback control of the Dicke-Hepp-Lieb superradiant quantum phase transition — •Wassilij Kopylov[1], Clive Emary[2], Eckehard Schöll[1], and Tobias Brandes[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin — [2]Department of Physics and Mathematics, University of Hull, United Kingdom

We apply the time-delayed Pyragas control scheme to the dissipative Dicke system, modulating it by the difference of photon numbers emitted from the cavity. Using the mean field approach and linear stability analysis we show that this control dramatically affects the states in the primary superradiant regime, creating new limit cycle phases and a rich phase diagram. We also derive an analytical transcendental equation for the boundaries between the different zones in the phase diagram.

DY 5.6 Mon 17:00 HÜL 186

Time-delayed control of (un)stable steady states in open quantum systems — •Philipp Strasberg and Tobias Brandes — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany

We consider the quantum version of classical time-delayed feedback to control (un)stable steady states of a quantum system. The system is then described by a (non-linear) stochastic master equation, which can be mapped to a set of time-delayed stochastic differential equations for the means and a set of a non-linear equations for the covariances. At steady state, the equations for the means are on average the same as for the classical case with a stochastic part coming purely from the quantum measurement and feedback.

Invited Talk DY 5.7 Mon 17:15 HÜL 186

Feedback control in quantum transport — •Clive Emary — Department of Physics and Mathematics, University of Hull, United Kingdom

Quantum transport is the study of the movement of electrons in structures small enough that the quantum properties of the electron play an important role. Recent "full counting statistics" experiments provide detailed time-resolved information on the stochastic motion of electrons in such structures which, it is proposed, could form the basis of feedback control schemes for quantum transport. Such feedback control has been shown to give rise to many interesting effects such as the suppression of unwanted current fluctuations, the realisation of a nanoelectric Maxwell's daemon and the stabilisation of non-equilibrium pure states.

In this talk I will review these proposals and discuss the effects of delay on such quantum feedback schemes. I will conclude with some perspectives on the use of coherent — as opposed to measurement-based — quantum control strategies in the transport setting.

DY 6: Statistical Physics far from Thermal Equilibrium - Part II

Time: Monday 15:00–17:30 Location: ZEU 160

Invited Talk DY 6.1 Mon 15:00 ZEU 160

Odd Bose condensation far from equilibrium — Daniel Vorberg[1,2], Waltraut Wustmann[1,2], Roland Ketzmerick[1,2], and •André Eckardt[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, 01187 Dresden, Germany

Bose-Einstein condensation, the macroscopic occupation of a single quantum state, appears in equilibrium quantum statistical mechanics. We show that even when a degenerate Bose gas is driven into a steady state far from equilibrium, e.g. by time-periodic driving, Bose-Einstein condensation survives in a generalized form [1]: the unambiguous selection of an odd number of states acquiring large occupations.

We study the effect in driven-dissipative model systems and propose a quantum switch for heat conductivity based on shifting between one and three *Bose selected* states.

[1] D Vorberg, W Wustmann, R Ketzmerick, and A Eckardt, Phys. Rev. Lett. **111**, 240405 (2013)

DY 6.2 Mon 15:30 ZEU 160

Superfluid Turbulence, Vortex Dynamics, and Universality in Ultracold Bose Gases — •Markus Karl[1,2], Boris Nowak[1,2], and Thomas Gasenzer[1,2] — [1]Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg — [2]ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt, Germany

Inspired by turbulence in classical hydrodynamics great efforts have been made in recent years to investigate and describe its quantum analogon in superfluids such as Helium and Bose–Einstein condensates. Here the intriguing difference to classical turbulence is that vortical flows can appear only quantised and are carried by particle-like excitations, namely vortices. Nevertheless, characteristic scaling laws for the kinetic energy appear also in quantum turbulent systems, establishing a notion of universality similar to Kolmogorov turbulence in classical hydrodynamics. In this talk we discuss quantum turbulence in far-from-equilibrium Bose gases as a result of interacting vortices and tangles of vortex lines. The emergence of universal scaling laws for the kinetic energy and the occupation spectrum respectively, $n(k) \sim k^{-\zeta}$, is demonstrated using semi-classical simulations and explained with the intrinsic scaling properties of the building blocks of quantum turbulence, *i.e.* the vortices. In addition the occupation spectra for the dynamically evolving Bose gas are analysed using quantum-field theoretic methods based on effective-action techniques. This approach leads to a close connection between steady universal scaling solutions and stationary fluxes of energy or particles in momentum space.

DY 6.3 Mon 15:45 ZEU 160

Heat transport through spin chains — •Gernot Schaller[1], Malte Vogl[2], and Tobias Brandes[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Max-Planck-Institut für Physik Komplexer Systeme, Dresden, Germany

Starting from microscopic spin-boson-type models we compare the heat transport through closed and open spin chains with and without disorder. Extending previous work [1] we calculate transport characteristics via locally coupling two heat reservoirs to the spin chain. Since for the closed spin chain many degeneracies are present, we compare results from the full quantum master equation approach with results from the rate equation approach. In both cases we find that transport is strongly dependent on the phase of the spin chain.

[1] M. Vogl, G. Schaller, and T. Brandes, PRL **109**, 240402 (2012).

DY 6.4 Mon 16:00 ZEU 160

Thermodynamics of Quantum-Jump-Conditioned Feedback Control — •Philipp Strasberg[1], Gernot Schaller[1], Tobias Brandes[1], and Massimiliano Esposito[2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany — [2]Complex Systems and Statistical Mechanics, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We consider open quantum systems weakly coupled to thermal reservoirs and subjected to quantum feedback operations triggered with or without delay by monitored quantum jumps. We establish a thermodynamic description of such systems and analyze how the first and second law of thermodynamics are modified by the feedback. We apply our formalism to study the efficiency of a qubit subjected to a quantum feedback control and operating as a heat pump between two reservoirs. We also demonstrate that quantum feedbacks can be used to stabilize coherences in nonequilibrium stationary states which in some cases may even become pure quantum states.

Ref.: arXiv:1305.6589 (accepted by Phys. Rev. E)

DY 6.5 Mon 16:15 ZEU 160

Quantum critical temperature of a modulated oscillator — Lingzhen Guo[1], Vittorio Peano[2], •Michael Marthaler[1], and Mark Dykman[3] — [1]Institut für Theoretische Festkörperphysik, KIT, Karlsruhe — [2]Institute for Theoretical Physics II, University of Erlangen-Nuremberg, Erlangen — [3]Department of Physics,Department of Physics and Astronomy, Michigan State University, East Lansing

We show that the rate of switching between the vibrational states of a modulated nonlinear oscillator is characterized by a quantum critical temperature $T_c \propto \hbar^2$. The rate is independent of T for $T < T_c$. Above T_c there emerges a quantum crossover region where the slope of the logarithm of the distribution over the oscillator states displays a kink and the switching rate has the Arrhenius form with the activation energy independent of the modulation. The results demonstrate the limitations of the real-time instanton theory of switching in systems lacking detailed balance.

15 min break

DY 6.6 Mon 16:45 ZEU 160

Observable most probable trajectories of quantum switching in modulated oscillator — •Vittorio Peano[1] and Mark Dykman[2] — [1]Friedrich Alexander Universität Erlangen — [2]Michigan State University

Quantum fluctuations lead to a finite width of the distribution of a modulated system over its quasienergy (Floquet) states even for zero temperature of the bath to which the system is coupled. We study the resulting distribution for a periodically modulated oscillator. Of special interest are large rare fluctuations responsible for the tail of the distribution over quasienergy and for switching between metastable states of forced vibrations. We find the most probable paths followed by the quasienergy in rare events, including switching. Along with the switching rates, such paths are observable characteristics of quantum fluctuations. As we show, they can change discontinuously once the detailed balance condition is broken (leading to the quantum crossover discussed in [1]). Knowledge of such paths suggests a new way of quantum control of rare events.

[1] see M. Marthaler contribution

DY 6.7 Mon 17:00 ZEU 160

Elektronischer Energietransport in Metallen fernab vom thermischen Gleichgewicht — •Orkhan Osmani, Mourad El Kharrazi und Marika Schleberger — Universität Duisburg-Essen, Fakultät für Physik

Formal lässt sich der Energietransport mittels kinematischer Modelle wie der Monte Carlo Methode oder der Boltzmanngleichung beschreiben, wobei der mikroskopische Zustand des Systems durch die Orte und Impulse aller Teilchen definiert wird. In solchen Modellen müssen für die zeitliche Entwicklung eines mikroskopischen Systems charakteristische Größen wie Stoßraten für alle physikalischen Prozesse, wie z.B. Elektron-Elektron oder Elektron-Phonon Stöße, explizit bekannt sein. Jedoch sind solche Modelle durch den hohen numerischen Aufwand oft ungeeignet, große Systeme unter vertretbarem Zeitaufwand zu beschreiben. Eine häufig verwendete Vereinfachung ist es, den Transport mittels einer Wärmeleitungsgleichung zu beschreiben, so dass der Zustand nun makroskopisch durch die Temperatur definiert ist. Hierbei ist die zeitliche Entwicklung des Systems durch die Wärmekapazität und Wärmeleitfähigkeit gegeben. Während der Übergang vom mikroskopischen zur makroskopischen Beschreibung für den Fall einer Gleichgewichtsverteilungsfunktion immer möglich ist, ist der Übergang für eine Nichtgleichgewichtsverteilung fragwürdig. Um diese Frage zu klären, haben wir den Energietransport in Metallen für verschiedene Nichtgleichgewichtsverteilungen mittels der Boltzmanngleichung, unter Berücksichtigung der El.-El.-Stöße, untersucht und anschließend mit einer Wärmeleitungsgleichung verglichen.

DY 6.8 Mon 17:15 ZEU 160

Formation of correlations at short time scales — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP), Avenida Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Using a conserving relaxation-time approximation an analytic formula is derived which describes the time dependence of the formation of correlations in two distinct physical systems: (i) the collective modes in a plasma created by a short intense laser pulse with an additional external electric field bias reproducing experimental universal features of the transient time behaviour of femtosecond spectroscopy (Phys. Rev. B 72 (2005) 233203) and (ii) the population dynamics of cold atomic gases on an optical lattice after a sudden quench.

DY 7: Glasses (joint session DY/ DF/ CPP)

Time: Monday 15:00–17:30 Location: ZEU 146

DY 7.1 Mon 15:00 ZEU 146

Dynamic Crossover and Stepwise Solidification of Confined Water — •Matthias Sattig and Michael Vogel — Hochschulstraße 6, D-64289 Darmstadt

The dynamical behaviour of water in the regime of the supercooled liquid is still a topic of large interest. In particular, the existence of a fragile-to-strong transition (FST) at around 225K induced by a liquid-liquid phase transition (LL) is controversially discussed [1]. The proposed temperature range of the FST is hardly accessible in bulk water.

Our ^{2}H NMR investigation reveals two dynamic crossovers of supercooled water in nanoscopic (nm) confinement. A dynamic crossover of liquid water at ca. 225K is accompanied by a formation of a fraction of solid water. Therefore, this effect can not be attributed to the LL, but rather to a change from liquid-like to interface-dominated dynamics. Moreover, the ^{2}H NMR data yield evidence that the α process and β process are observed in experiments above and below this temperature, respectively. Upon cooling through a dynamic crossover at ca. 175K, the dynamics of the liquid fraction becomes anisotropic and localized, implying solidification of the corresponding water network, most probably, during a confinement-affected glass transition.

[1] Mishima; Nature, Vol. 396, 329(1998)

DY 7.2 Mon 15:15 ZEU 146

Understanding the nonlinear mobility of single driven particles in supercooled liquids — •Carsten F. E. Schroer[1,2] and Andreas Heuer[1,2] — [1]WWU Münster, Münster, Germany — [2]Graduate School of Chemistry, Münster, Germany

We perform MD simulations of a binary Lennard-Jones mixture where a single particle is pulled by an external field through the liquid. Herein, we are specifically interested in the range of intermediate and strong forces when nonlinear effects occur in the single particle dynamics.

It is known from experimental and simulation studies, that the steady-state velocity $\overline{v}$ follows in the limit of low forces a linear response relation $\overline{v} = \mu F$ where the force F is connected to the dynamical response via the constant mobility $\mu_0 = \frac{D_0}{k_B T}$. For large forces, however, one finds a dramatic increase of $\overline{v}$ with increasing F, indicating a nonlinear force-dependence of the mobility, i.e. $\mu_0 \to \mu(F)$.

To gain a deeper understanding of this behavior, we studied the underlying potential energy landscape of the system by computing the minima the system has resided in during its time-evolution. This immediately allows us to discuss the nonlinear mobility in terms of thermodynamical (distribution of energies) and kinetic (escape rates out of single minima) quantities. Most interestingly it turns out, that

both effects are of major importance for the nonlinearity of the system, so that there is no single nonlinear effect but an interplay of two independent which contributes to the dynamical responses of the driven particles.

DY 7.3 Mon 15:30 ZEU 146

Simulation of Borate glasses — •Christoph Scherer[1,2], Friederike Schmid[1], Martin Letz[2], and Jürgen Horbach[3] — [1]Johannes Gutenberg-Universität, Mainz — [2]Schott AG, Mainz — [3]Heinrich-Heine-Universität, Düsseldorf

The model glass former B2O3 is studied as an example for generating accurate glass structures on the computer. B2O3 is an important component for the simulation of oxide glasses since boron can form triangular planar structures, as well as tetrahedral nearest neighbor structures and also boroxol rings. In one approach, configurations of a few hundred atoms are equilibrated at high temperature, well above the glass transition temperature, with a classical molecular dynamics simulation (MD). After a quench down to 0K, they are structurally relaxed by means of an ab inito (DFT) calculation. The structural and vibrational properties are compared to the results of a full ab inito quench to 0K and to experimental results. The dependence of the glass structure and the liquid properties on the classical force field is examined. Therefore, a set of classical force fields is generated by means of a structural fitting procedure. The parameters are fitted in a way that the structure, namely the radial distribution functions and the angular distributions, of a classical MD run matches as closely as possible the structure of an ab initio (DFT) run at the same temperature. Parameter fits are carried out according to an ab initio trajectory at high temperature, where the system is in the liquid state. This sets the basis for the next steps: The development of a classical force field for sodium-borate glasses by the same methodology.

DY 7.4 Mon 15:45 ZEU 146

Mixing random organization and jamming — •Michael Schmiedeberg — Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40204 Düsseldorf, Germany

The random organization and the athermal jamming transition can both be studied in a unifying model system. We study the mixture of the protocols of the two transitions and argue that such a mixture can be interpreted as the glass transition at small but non-zero temperatures.

In our model system, first particles are randomly distributed and then in each step overlapping particles are displaced. In case of displacements in random directions the so-called random organization transition is observed. For purely deterministic displacements the jamming transition is realized. While the jamming protocol match with a quench of a soft sphere system from infinite to zero temperature without crossing energy barriers, the random displacements of the random organization protocol correspond to thermally activated rearrangements of particles. If in a mixed protocol the probability of random displacements is small but non-zero we find that the transition differs significantly from the purely deterministic jamming transition. We believe that our model system can help to understand why there is a difference between the glass transition at small but non-zero temperatures and the athermal jamming transition.

DY 7.5 Mon 16:00 ZEU 146

Existence of glass-form factors — •Thomas Franosch — Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, A-6020 Innsbruck, Austria

A hallmark of the glass transition is the slow structural relaxation of a quasi-arrested structure. As an idealization the dynamics is considered to become non-ergodic directly at the glass transition such that all auto-correlation function coupling to the structural relaxation exhibit finite non-trivial long-time limits often referred to as glass-form factors or nonergodicity parameters. Simultaneously, the theory of stochastic processes in the framework of probability theory imposes quite stringent conditions on the class of correlation functions. The existence of a finite limit at long times is then connected to the properties of the associated spectral measure, and in general correlation functions can either oscillate forever, display quasi-periodic behavior, or even intermittent behavior. While for purely relaxation dynamics, e.g. Brownian dynamics, the existence of a long-time limit is trivial, the situation for the case of Newtonian dynamics has been elusive so far.

In this talk I elaborate conditions covering a broad class of theoretical approaches that guarantee the existence of a long-time limit. As a special case I show that the mode-coupling theory of the glass transition belongs to that class. As an outlook I briefly discuss the case of multiple decay channels relevant for molecular or confined systems.

15 min break

DY 7.6 Mon 16:30 ZEU 146

Spin freezing in geometrically frustrated magnets — Jorge Rehn[1], Arnab Sen[1,2], •Alexei Andreanov[1], Antonello Scardicchio[3], Kedar Damle[4], and Roderick Moessner[1] — [1]Max-Planck Institut fur Physik komplexer Systeme, Dresden, Germany — [2]Indian Association for the Cultivation of Science, Kolkata, India — [3]The Abdus Salam ICTP, Trieste, Italy — [4]The Tata Institute, Mumbai, India

Materials which are believed to be faithfully represented by classical frustrated magnets with macroscopically degenerate groundstates, often exhibit spin-freezing. The latter is a transition to a spin-glass phase. Explaining the mechanism of such freezing is not always a simple task, since conventional ingredients, like randomness of the interactions, is not always present in the systems under study. We present a model, where dilution alone generates frustrating interaction between certain spins in the systems and leads to their freezing. The effective model deals with antiferromagnetically coupled Heisenberg spins in 2D. Both the long-range nature of the interaction and its dependence on the distance are crucial for the existence of the glass phase. We confirm our predictions by performing Monte-Carlo simulation of the effective model.

DY 7.7 Mon 16:45 ZEU 146

Glasses of binary colloidal mixtures in the quiescent state and under shear — •Tatjana Sentjabrskaja, Marco Laurati, and Stefan Egelhaaf — Condensed Matter Physics Laboratory, Heinrich-Heine Universität Düsseldorf, D-40225 Düsseldorf, Germany

We investigate mixing effects on the glass state of binary colloidal hard sphere mixtures with large size asymmetry (size ratio 1:5). Increasing the amount of small spheres in a system of large ones, a glass-glass transition is observed, where the large particles, initially caged by the large spheres, become localised in a cage of small spheres [1]. During the transition, the dynamics accelerate and a strong reduction of the yield strain as a result of the shift of random close packing is observed[2].

The results of rheology are compared to measurements of the dynamics of particles under shear. The super-diffusion typically associated with stress overshoots [3] becomes more pronounced for mixtures in which the dynamics are increasingly arrested. Moreover, we observe different degrees of shear-induced constriction depending on mixing ratio, which closely follow changes in the magnitude of the stress overshoot.

[1] T.Sentjabrskaja et al., AIP Conf.Proc., 1518, 206, 2013.
[2] T.Sentjabrskaja et al., Soft Matter, 9(17), 4524- 4533, 2013.
[3] M.Laurati et al., J. Phys.: Condens. Matter, 24, 464104, 2012.

DY 7.8 Mon 17:00 ZEU 146

Microscopic theory for sheared colloidal glasses and gels — •Christian Amann and Matthias Fuchs — Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

We use mode coupling theory (MCT) to calculate in three dimensions (3D) transient density autocorrelators in start-up shear flow. It is thus possible to quantitatively predict flow curves and distorted structure of colloidal glasses and gels under shear flow. We investigate the transient, non-linear, non-monotonous stress response to strain and structure-factor distortion in 3D as well as steady-state flow curves (cf. [1] for 2D calculations). Density correlators, stress response, and structure-factor distortions are in good qualitative agreement with experiments [2], while the quantitative errors of the theory can be identified. A close connection between the time-evolution of symmetries of structure-factor distortions and non-monotonous stress response (i.e. stress overshoot) can be observed. We use as input a structure factor calculated with analytical Percus Yevick closure, which allows to approximate a hard sphere repulsion as well as augmenting a short range square-well attraction [3]. Hence, implications of a gel-glass to repulsive-glass transition on the transient rheology can be studied.

[1] Amann, C.P. et al. *J. Rheol.* **57**, 149 (2013); Henrich O. et al. *Phil. Trans. R. Soc. A* **367**, 5033 (2009)
[2] Denisov, D. et al. *Sci. Rep.* **3**, 1631 (2013)
[3] Dawson K. et al. *PRE* **63**, 011401 (2000)

DY 7.9 Mon 17:15 ZEU 146

An efficient Monte Carlo algorithm to study structural relaxation in network forming materials — •Richard Vink — Institute of Theoretical Physics, Georg-August-Universität Göttingen, Germany

Network forming materials are ubiquitous in nature, common examples being semiconductors such as silicon and silica, as well as fluids that can form hydrogen bonds. What these materials have in common is that their topology on short length scales is governed by certain rules. For example, in amorphous silicon, most atoms are 4-fold coordinated, the preferred Si-Si bond length being $\approx$ 2.35 Å, and the preferred Si-Si-Si bond angle being the tetrahedral angle. This complicates molecular dynamics simulations of these materials, where the particles spend most of their time thermally fluctuating about their equilibrium positions, while large structural changes in the network topology are rare. To overcome this problem, Wooten, Winer, and Weaire (WWW) introduced a special Monte Carlo move consisting of bond switching Monte Carlo moves which turned out to be very efficient at structurally relaxing networks of amorphous silicon and silica [Phys. Rev. Lett. **54** 1392 (1985)]. Unfortunately, the algorithm is only correct when used at zero temperature. In order to also address finite temperature, I propose a modification to the original WWW algorithm such that the Boltzmann distribution is faithfully sampled at any given temperature. The resulting algorithm is used to study the melting transition of a two-dimensional three-fold coordinated network.

DY 8: Critical Phenomena and Phase Transitions

Time: Monday 15:00–18:15 Location: ZEU 118

DY 8.1 Mon 15:00 ZEU 118

Corner contribution to cluster numbers in the Potts model — Istvan A. Kovacs[1], Eren M. Elçi[2], •Martin Weigel[2], and Ferenc Igloi[1] — [1]Wigner Research Centre, Institute for Solid State Physics and Optics, H-1525 Budapest, P.O.Box 49, Hungary — [2]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England

For the two-dimensional Q-state Potts model at criticality, we consider Fortuin-Kasteleyn and spin clusters and study the average number N_Γ of clusters that intersect a given contour Γ. To leading order, N_Γ is proportional to the length of the curve. Additionally, however, there occur logarithmic contributions related to the corners of Γ. These are found to be universal and their size can be calculated employing techniques from conformal field theory. For the Fortuin-Kasteleyn clusters relevant to the thermal phase transition we find agreement with these predictions from large-scale numerical simulations. For the spin clusters, on the other hand, the cluster numbers are not found to be consistent with the values obtained by analytic continuation, as conventionally assumed.

DY 8.2 Mon 15:15 ZEU 118

Fragmentation of Potts clusters — •Eren M. Elçi and Martin Weigel — Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England

The random cluster model is at the heart of a range of models in statistical physics, including uniform spanning trees, percolation and the Potts model. Many geometric and fractal aspects have been analysed, in particular at criticality, and a related zoo of exponents is known exactly or at least accessible by numerical methods. The fragmentation of clusters is a process of general importance for the modeling of a wide range of phenomena, including polymer fragmentation and processes in porous media. We use extensive numerical simulations employing a recent efficient implementation of Sweeny's single-bond algorithm to study the distribution of cluster sizes as well as the density of fragmenting (or bridge) bonds relevant to the fragmentation properties. The latter quantity is of additional importance for algorithmic aspects such as the observed critical speeding up of the single-bond dynamics.

DY 8.3 Mon 15:30 ZEU 118

Simulated tempering and magnetizing Monte Carlo study of crossover scaling in the 2d 3-state Potts model — Tetsuro Nagai[1], Yuko Okamoto[1], and •Wolfhard Janke[2] — [1]Department of Physics, Nagoya University, Nagoya, Aichi 464-8602, Japan — [2]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

The recently introduced simulated tempering and magnetizing (STM) Monte Carlo method is a variant of generalized ensemble algorithms that aims at covering a mesh of simulation points in the two-dimensional temperature-field plane in a dynamically controlled manner. We applied STM Monte Carlo simulations to the two-dimensional three-state Potts model in an external magnetic field in order to investigate the crossover scaling behaviour in the temperature-field plane at the Potts critical point and towards the Ising universality class for negative magnetic fields. Our data set has been generated by STM simulations of several square lattices with sizes up to 160×160 spins, supplemented by conventional canonical simulations of larger lattices at selected simulation points. Careful scaling and finite-size scaling analyses of the crossover behaviour with respect to temperature, magnetic field and lattice size will be discussed.

T. Nagai, Y. Okamoto, and W. Janke, J. Stat. Mech.: Theor. Exp. (2013) P02039; Condens. Matter Phys. **16** (2013) 23605.

DY 8.4 Mon 15:45 ZEU 118

Non-equilibrium box overlap in spin glasses — •Markus Manssen[1], Alexander K. Hartmann[1], and A. Peter Young[2] — [1]Carl-von-Ossietzky Universität Oldenburg, Germany — [2]University of California, Santa Cruz, USA

One of the most prominent questions in the theory of spin glasses is the extent to which the mean field solution applies in more realistic situations such as three dimensions. Although not all properties of the mean field solution are reproduced in in three-dimensional systems, numerical simulations indicate that the distribution $P(q)$ of spin overlaps does resemble that in mean field theory, and the same seems to hold for overlaps in small cubic boxes of side length B. Here we have studied box overlaps in the non-equilibrium regime to investigate what changes occur when the range of correlations, initially very small, grows with time and eventually exceeds the box size. We performed long time simulations over 10^8 time steps of the 3D Edwards-Anderson model of size 128^3 with binary couplings by utilizing general purpose GPU programming, which allows us to reach single-spin-flip times of 8ps. We measured the growing correlations and box overlaps. Additionally we simulated smaller systems to see what changes in the box overlaps occur when the whole system equilibrates.

DY 8.5 Mon 16:00 ZEU 118

Self-avoiding walks and Θ-polymers on crititcal percolation clusters — •Niklas Fricke and Wolfhard Janke — Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ), Universität Leipzig, Postfach 100920, 04009 Leipzig, Germany

Self-avoiding walks (SAWs) on critical percolation clusters are a basic model for polymers in crowded disordered media. The fractal nature of the clusters gives rise to interesting scaling behavior of the SAWs, which is still poorly understood despite considerable efforts in the past. We developed an exact enumeration method which exploits the fractal structure of the critical cluster [1]. The method can handle walks of several thousand steps, amounting to over 10^{1000} conformations. This enables us to determine the SAW scaling exponents on critical percolation clusters with unprecedented accuracy. We also look at self-attracting SAWs, a.k.a. Θ-polymers. Here, the comprehensive information obtained via exact enumeration is particularly valuable as it allows for a close analysis of temperature-driven phase transitions.

[1] N. Fricke and W. Janke, Europhys. Lett. 99, 56005 (2012).

DY 8.6 Mon 16:15 ZEU 118

News and views in discontinuous phase transitions — •Jan Nagler — ETH Zurich

Recent progress in the theory of discontinuous percolation allows us to better understand the the sudden emergence of large-scale connectedness both in complex networked systems and on the lattice. We analytically study mechanisms for the amplification of critical fluctuations at the phase transition point, non-self-averaging and power law

fluctuations. 'Single event analysis' allows to establish criteria for discontinuous percolation transitions, even on the high-dimensional lattice. Some applications such as salad bowl percolation, competitive establishment of links in growing networks, crackling noise and inverse fragmentation are discussed.

15 min break

Invited Talk DY 8.7 Mon 16:45 ZEU 118

Self-organized criticality in Hamiltonian spin systems: intriguingly ordinary or ordinarily intriguing? — •Helmut G. Katzgraber — Texas A&M University, USA

Self-organized criticality (SOC) refers to the tendency of dissipative systems to drive themselves into a scale-invariant critical state without any parameter tuning. These phenomena are of crucial importance because fractal objects displaying SOC are found everywhere, e.g., in earthquakes, the meandering of sea coasts, or in galactic clusters. Understanding its origin, however, represents a major unresolved puzzle. Pioneering work in the 1980s provided insights into the possible origins of SOC: The sandpile and forest-fire models are hallmark examples of dynamical systems that exhibit SOC. However, these models feature ad hoc dynamics, without showing how these can be obtained from an underlying Hamiltonian. The possible existence of SOC was also tested in random magnets, such as the random-field Ising model, but in all these, at least one parameter had to be tuned, i.e., no true SOC. The first Hamiltonian model displaying true SOC was the infinite-range mean-field Sherrington-Kirkpatrick spin-glass model. Here, we investigate the conditions required for general disordered magnets to display self-organized criticality. Our results are in disagreement with the traditional lore that self-organized criticality is a property of the mean-field regime of spin glasses. In fact, self-organized criticality is recovered only in the strict limit of a diverging number of neighbors. In light of these result, the behavior of damage spreading on scale-free networks, as well Coulomb glasses are discussed.

DY 8.8 Mon 17:15 ZEU 118

Dynamic scaling and superdiffusion in a critical binary mixture — Dipanjan Chakraborty[1,2], Siegfried Dietrich[1], and •Felix Höfling[1] — [1]Max Planck Institute for Intelligent Systems, Stuttgart, and Institute for Theoretical Physics IV, Universität Stuttgart, Germany — [2]IISER Mohali, SAS Nagar, India

A binary mixture near its consolute point exhibits critical fluctuations of the local composition. The static properties of the mixture are well described by the 3D Ising universality class [1], the dynamic properties involving conservation of particles, energy, and momentum are classified as *model H′*. So far, theoretical work on the critical dynamics has focused on transport coefficients, while studies of the relaxation dynamics of the spatially resolved order parameter are missing.

We present numerical results for the dynamic structure factor $S(k,t)$ of a symmetric binary Lennard-Jones mixture near its demixing transition. Employing the computing resources of high-end GPUs [2], we have performed microcanonical molecular dynamics simulations which cover system sizes of up to 216,000 particles and 4 non-trivial orders of magnitude in time. We explore the crossover of the k-dependent relaxation time from diffusion-like to critical behaviour and find nice agreement with theoretical predictions. Dynamic scaling of $S(k,t)$ at criticality is tested and scaling functions are deduced. For interdiffusion, we have evidence that the vanishing of the diffusion constant is accompanied by *super*diffusion within intermediate time windows.

[1] S. K. Das *et al.*, J. Chem. Phys. **125**, 024506 (2006)

[2] P. Colberg and F. Höfling, Comp. Phys. Comm. **182**, 1120 (2011)

DY 8.9 Mon 17:30 ZEU 118

Numerical evidence for strong randomness scaling at a superfluid-insulator transition of one dimensional bosons — •Susanne Pielawa[1] and Ehud Altman[1,2] — [1]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — [2]Department of Physics, University of California, Berkeley, California 94720, USA

We present numerical evidence from Monte-Carlo simulations that the superfluid-insulator quantum phase transition of interacting bosons subject to strong disorder in one dimension is controlled by the strong-randomness critical point. At this critical point the distribution of superfluid stiffness over disorder realizations develops a power-law tail reflecting a universal distribution of weak links. The Luttinger parameter on the other hand does not take on a universal value at this critical point, in marked contrast to the known Berezinskii-Kosterlitz-Thouless-like superfluid-insulator transition in weakly disordered systems. We develop a finite-size scaling procedure which allows us to directly compare the numerical results from systems of linear size up to 1024 sites with theoretical predictions obtained in [PRL 93, 150402 (2004)], using a strong disorder renormalization group approach. The data shows good agreement with the scaling expected at the strong-randomness critical point.

DY 8.10 Mon 17:45 ZEU 118

Universal shape functions at classical critical points — •Stephen Inglis[1], Jean-Marie Stèphan[2], Paul Fendley[2], and Roger G. Melko[1,3] — [1]University of Waterloo, Waterloo, Canada — [2]University of Virginia, Charlottesville, USA — [3]Perimeter Institute for Theoretical Physics, Waterloo, Canada

We demonstrate how the Rènyi mutual information (RMI) can be used to characterize universality at the critical point of two dimensional classical systems through their shape dependence, similar to the result of c-theorems in one dimensional systems.

We introduce a highly efficient method for calculating the RMI in discrete classical systems, and use it on the two dimensional Ising and Potts models. This method avoid the difficulty of thermodynamic integration needed in earlier techniques [Phys. Rev. B 87, 195134 (2013)] and allows for direct access to the RMI for different geometries. The method is similar to the quantum ratio trick [Phys. Rev. Lett. 104, 157201 (2010)] except that we gain a large increase in speed and convergence by using classical Monte Carlo. In the cases where classical critical points contain the universality class of interest, this method represents a more efficient approach for extracting universal shape functions.

DY 8.11 Mon 18:00 ZEU 118

Queue with exclusion — •Chikashi Arita[1] and Andreas Schadschneider[2] — [1]Theoretische Physik, Universität des Saarlandes, Saarbrücken, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Köln, Germany

The history of the queueing theory goes back to A K Erlang 1909. The M/M/1 queueing process is one of basic models in which injection and extraction of particles (customers) are imposed. When pedestrians make a queue, they usually proceed when there is a space in front of them. However this excluded-volume effect is neglected in the M/M/1 queue. The "exclusive queueing process (EQP)" was introduced to take this effect into account by imposing a new boundary condition on the exclusion process [1,2]. The M/M/1 queue converges (diverges) when the incoming rate is smaller (greater) than the outgoing rate, "phase transition". On the other hand, in the EQP, the incoming rate is restricted by the so-called maximal current of the exclusion process for convergence, i.e. "the queue itself is a bottleneck." This property was derived by using an exact stationary state [1,2]. Furthermore, with helps of Monte Carlo Simulations, some time dependent properties of the system length L have been investigated [3,4,5]. Recently an update rule dependent behavior of L was found on the phase transition line [6].

[1] CA: Phys Rev E 80, 051119 (2009) [2] CA & D Yanagisawa: J Stat Phys 141, 829 (2010) [3] CA & AS: Phys Rev E 83, 051128 (2011) [4] CA & AS: Phys Rev E 84, 051127 (2011) [5] CA & AS: J Stat Mech, P12004 (2012) [6] CA & AS: EPL, in press (2013)

DY 9: Focus Session: Dynamical Patterns in Neural Systems: From Brain Function to Dysfunction (joint session DY/ BP)

Pattern formation in biological systems is at the forefront of current cross-disciplinary research; scientists are striving across disciplines to understand detailed activity patterns in neural systems and their role in brain function.This focus session will outline the potential of modern imaging and network approaches for revealing collective mechanisms underlying normal and pathophysiological activity in the brain. (Organizers St. C. Müller and Th. Geisel)

Time: Tuesday 9:30–11:30 Location: HÜL 186

Invited Talk DY 9.1 Tue 9:30 HÜL 186

From epilepsy to migraine to stroke: A unifying framework. — •Markus A Dahlem — Department of Physics, Humboldt-Universität zu Berlin

We seek to understand in terms of quantitative mathematical models the dynamics of ion imbalances in three pathological conditions: epileptiform activity during seizures, cortical spreading depression in migraine, and anoxic depolarizations after stroke or traumatic brain injury. A family history of epilepsy increases the chances of having severe migraines and certain patients with migraine are at greater risk for stroke. The multiplicity of potential links include common genetic risk factors and indirect links like common triggers outside the brain. In the present approach, however, we will focus on basic electrophysiological mechanisms of neural excitability and the transitions between different activity forms related to ion imbalances in the brain. The change of both membrane potential and—due to reduced ion gradients—Nernst potentials together cause in varying degrees a release of Gibbs free energy, that is, the thermodynamic potential that measures the energy available to the neurons for normal functioning. We hence describe the three states related to epilepsy, migraine, and stroke in terms of their free energy starvation and stress. The mathematical description of such phenomena requires a broader thermodynamical perspective, as it goes beyond the original Hodgkin-Huxley description based on equivalent electrical circuits in membrane physiology.

Invited Talk DY 9.2 Tue 10:00 HÜL 186

Non-standard Interactions in Networks: Synchrony and the Emergence of Neural Activity Patterns — •Marc Timme[1], Sven Jahnke[1], Raoul-Martin Memmesheimer[2], Wen-Chuang Chou[1], and Christian Tetzlaff[1] — [1]Network Dynamics, MPI for Dynamics and Self-Organization — [2]Donders Institute for Neuroscience, University of Nijmegen

Patterns of spatio-temporally distributed neural activity have been experimentally observed in different systems and are intimately related to network function. How spatial and temporal specificity emerge dynamically in neural circuits, however, remains unclear.

Here we demonstrate how non-standard interaction mechanisms such as non-additive coupling and inhibitory feedback co-acting with heterogeneities may generate apparently disordered patterns that yet are precise in space and time and selectively respond to specific inputs only. The results may contribute towards an explanation of sensory processing in olfactory systems and processes involved in memory consolidation.

References: PLoS Comput. Biol. 8:e1002384 (2012); Phys. Rev. X 2:041016 (2012); PLoS Comput. Biol. 9:e1003307 (2013); Chou et al., in prep.

Invited Talk DY 9.3 Tue 10:30 HÜL 186

Towards a dynamic map of neuronal circuits — •Alipasha Vaziri — Research Institute of Molecular Pathology (IMP), — Center for Molecular Biology, University of Vienna — Research Platform for Quantum Phenomena and Nanoscale Biological Systems, University of Vienna

Knowledge on structural connectivity in neuronal circuits is necessary for understanding information representation and processing in local circuits. Addressing this challenge has been hampered by lack of appropriate tools and methods that allow parallel and spatiotemporally specific application of excitation patterns onto neuronal populations while capturing the dynamic activity of the entire network at high spatial and temporal resolution. The combination of new optical excitation techniques, optogenetics and high speed functional imaging are providing new opportunities to address this question and move towards a dynamic map of neuronal circuits. Compared to standard two-photon microscopy exploiting the spectral properties of femtosecod lasers provide an additional degree of freedom whereby alternative spatial light distributions can be "sculpted" in a biological sample. We have developed such a two-photon technique for brain-wide calcium imaging in C. elegans. The combination of this microscope with a nuclear-localized, genetically encoded calcium indicator, NLS-GCaMP5K, has allowed us to capture the activity of individual neurons within the densely packed head ganglia of C. elegans. We demonstrate near-simultaneous recording of activity of up to 70% of all head neurons.

DY 9.4 Tue 11:00 HÜL 186

Fast reconfiguration of high-frequency human brain networks in response to surprising changes in auditory input — •Sandra Chapman[1,2,3], Ruth Nicol[4], Petra Vertes[5], Pradeep Nathan[5,6], Marie Smith[7], Yury Shtyrov[8], and Edward Bullmore[5,6] — [1]CFSA, Physics, Univ. of Warwick, UK — [2]MPIPKS, Dresden, Germany — [3]Mathematics and Statistics, UIT, Norway — [4]University Hospitals Coventry and Warwickshire NHS Trust, Coventry, UK — [5]Behavioral and Clinical Neuroscience Institute, Dept. of Psychiatry, Univ. of Cambridge, UK — [6]GSK Clinical Unit, Addenbrooke's Hospital, Cambridge, UK — [7]Dept. of Psychological Sciences, Birkbeck, Univ. of London, UK — [8]MRC Cognition and Brain Sciences Unit, Cambridge, UK

We measured rapid changes in functional brain network organization in response to brief, discrete, changes in auditori stimulii. We estimated network topology and distance parameters in the immediate response, < 1 s, following auditory presentation of standard, repeated tones interspersed with occasional 'surprising' tones, using MEG to measure synchronization of high frequency (gamma band 33-64 Hz) oscillations in healthy volunteers. We found that global small-world parameters of the networks were unchanged between the standard and surprising tones. However, auditory surprises were associated with local changes in clustering of connections between temporal and frontal cortical areas, and with increased interlobar, long-distance synchronization. This work maps the dynamic network response that corresponds to the well known evoked response to this mismatch-negativity paradigm.

DY 9.5 Tue 11:15 HÜL 186

The Cerebral Cortex as an Excitable Medium: Spiral Dynamics in Cortical Models of Epilepsy — •Kentaroh Takagaki — Leibniz Institut für Neurobiologie, Magdeburg, Germany

Epilepsy affects up to 50 million people worldwide, each year. Although much research has focused on the genetic and pharmacological aspects of this disorder, little is known about how the population activity patterns of neurons initiate and stabilize within the epileptic cortex. Our work in cortical slice models of epilepsy shows that spatially organized, dynamically stable spiral patterns may contribute to such epileptogenesis. We have also recently recorded such phenomena in vivo, in the Mongolian Gerbil.

We hypothesize that such spiral dynamics may serve a role similar to the well-known reentrant spirals in ventricular fibrillation of the heart. To explore this hypothesis and brain population dynamics in general, we have been applying transcranial DC stimulation to modulate the excitability of the cortex, and observing the resulting population dynamics via voltage-sensitive dye imaging.

DY 10: Nonlinear Stochastic Systems

Time: Tuesday 9:30–12:30 Location: ZEU 160

DY 10.1 Tue 9:30 ZEU 160

Fluctuation-Driven Shifts in Selection Regimes in Population Dynamics — •Yen Ting Lin[1], Hyejin Kim[2], and Charles Doering[3] — [1]Max Planck Institutes for the Physics of Complex Systems, Noetnitzer Str. 38, Dresden 01187 , Germany — [2]Department of Mathematics, Michigan State University, East Lansing, MI 48824, USA — [3]Department of Mathematics, University of Michigan, Ann Arbor, Michigan 48109-1043

Demographic stochasticity is an essential feature of population dynamics. Nevertheless theoretical investigations often neglect this naturally occurring noise due to the mathematical complexity of stochastic models. This talk reports the results of analytical and computational investigations of models of competitive population dynamics, specifically the competition between species in heterogeneous environments with different phenotypes of dispersal, fully accounting for demographic stochasticity. A novel asymptotic approximation is introduced and applied to derive remarkably simple analytical forms for key statistical quantities describing the populations' dynamical evolution. The theory is verified by conventional asymptotic analysis and large-scale numerical simulations. Both dynamical mechanisms and time scales of the fluctuation-induced phenomena are identified within the theoretical approach. The analysis highlights the fundamental physical effect of the fluctuations and provides an intuitive interpretation of the complex dynamics. An interaction between stochasticity and nonlinearity is the foundation of noise-driven dynamical selection.

DY 10.2 Tue 9:45 ZEU 160

Statistical classification of small microbial food webs — •Fanny Groll and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Germany

We identify classes of food webs with regard to their stability and species diversity. Food webs are characterised by the topology of their inter-species relations, e.g. feeding on products of metabolism of another species or competition on nutrients or via a common predator.

To gain insight into these structures we pursue a statistical approach: the starting point is the numerical implementation of food webs with given inter-species network dependence. Each species is defined by parameters determining its attributes. A whole distribution of parameter combinations is then randomly generated within biologically sensible bounds, and tested according to its temporal evolution. Individual systems evolve for some time in simulations and the outcome is monitored. Specifically, we deduce probabilities for the survival of a given number of species over distributions of network parameters at fixed network topology.

DY 10.3 Tue 10:00 ZEU 160

Stochastic switching in networks of delay-coupled oscillators — •Otti D'Huys[1], Thomas Juengling[2], and Wolfgang Kinzel[1] — [1]Institute for Theoretical Physics, University of Wuerzburg, 97074 Wuerzburg, Germany — [2]Instituto de Fisica Interdisciplinar y Sistemas Complejos, IFISC (UIB-CSIC), Campus Universitat de les Illes Balears, E-07122 Palma de Mallorca, Spain

Networks with coupling delays play an important role in various systems, such as coupled semiconductor lasers, traffic dynamics, communication networks, genetic transcription circuits or the brain . In oscillatory systems it is known that a delay induces multistability: the number of coexisting periodic orbits scales linearly with the coupling strength and the delay time.

Adding noise to the dynamics, the network switches between these coexistent orbits. For phase oscillator networks we construct a potential, which allows us to analytically compute the distribution of frequencies visited by the network and the corresponding residence times.

We find some surprising stochastic effects: with increasing delay the frequency distribution narrows, but the residence times are unaffected. With increasing coupling strength, the residence times in each orbit increase, but the number of attended orbits remains the same. Moreover, the network topology plays a crucial role: while in unidirectional rings in-phase and out-of-phase states are equally often attended, the out-of-phase states disappear for sufficiently long delays in most other networks.

DY 10.4 Tue 10:15 ZEU 160

Kolmogorov spectrum of renewable wind and solar power fluctuations — •Mehrnaz Anvari[1], Joachim Peinke[2], and Mohammad Reza Rahimi Tabar[3] — [1]ForWind and Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany — [2]ForWind and Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany — [3]ForWind and Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany

With increasing the contribution of renewable energies in power production, the task of reducing dynamic instability in power grids must also be addressed from the generation side, because the power delivered from such sources is spatiotemporally stochastic in nature.

Here we characterize the stochastic properties of the wind and solar energy sources by study their spectrum and multi-fractal exponents. The computed power spectrum from high frequency time series of solar irradiance and wind power reveals a power-law behavior with an exponent ˜ 5/3 (Kolmogorov exponent) in the frequency domain 0.001 Hz $<$ f $<$ 0.1Hz, which means that the power grid is being fed by turbulent-type sources.

DY 10.5 Tue 10:30 ZEU 160

Ultar-long-tail simulation and modelling of rogue wave statistics — Marc Eberhard[1], •Rudolf A. Römer[2], and Akihiro Maruta[3] — [1]Aston University, Birmingham, B4 7ET — [2]University of Warwick, Coventry CV4 7AL, UK — [3]Osaka University, 1-1 Yamadaoka, Suita, Osaka 565-0871, Japan

Optical "rogue waves" generated in fiber systems are sharp, rare and extremely high power pulses that share the main features of the devastating freak waves appearing in the ocean. In fact, rogue waves are known to occur also in plasmas, Bose-Einstein condensates and superfluid helium. Rogue waves are argued to to form due to at least two mechanisms of amplification. First, a modulation instability broadens the power spectrum of the waves - and hence "amplifies" waves in frequency ranges where there were none to start with. The second amplification is then due to multiple inelastic soliton collisions. In order to describe rogue waves quantitatively, it has been shown that their probability density function depicts a typical 'L-shaped' profile, characterizing the occurrence of many small events as well as, in the horizontal part of the 'L', some very rare and extremely powerful events. What drives the formation of this 'L'-shaped PDF is not yet clear. Recently, it was argued that a third-order dispersion term might be responsible. A remarkable feature of the third-order dispersion is that the energy of the stronger soliton in most of the cases increases after the collision. Hence after multiple such collisions, the strongest soliton will have accumulated most of the energy in the system, it has become a rogue wave!

DY 10.6 Tue 10:45 ZEU 160

Critical manifold and tricritical point of nonlinear globally coupled systems with additive noise — •Rüdiger Kürsten[1,2] and Ulrich Behn[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]International Max Planck Research School Mathematics in the Sciences, Leipzig, Germany

An infinite array of globally coupled overdamped constituents moving in a double-well potential under the influence of additive Gaussian white noise is closely related to a discretized version of the mean field φ^4-Ginzburg-Landau model. The system exhibits a continuous phase transition from a symmetric phase to a symmetry broken phase [1]. The qualitative behavior is the same for higher order saturation terms φ^n, where $n \geq 6$ is even. The critical point is calculated for strong and for weak noise, these limits are also bounds for the critical point. Introducing an additional nonlinearity, such that the potential can have up to three minima, leads to richer behavior. Then the parameter space divides in three regions, a region with a symmetric phase, a region with a phase of broken symmetry and a region where both phases coexist. The region of coexistence collapses into one of the others via a discontinuous phase transition whereas the transition between the symmetric phase and the phase of broken symmetry is continuous. The tricritical point where the three regions intersect, can be calculated for strong and for weak noise. These limiting values are the optimal bounds for the tricritical point.

[1] R. Kürsten, S. Gütter, U. Behn, Phys. Rev. E **88**, 022114 (2013)

15 min break

DY 10.7 Tue 11:15 ZEU 160

Dynamical complexity in noisy coupled cubic maps — •Thomas Zub and Stefan J. Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany

As far as its first bifurcation is concerned, the cubic map represents a discrete analogon to the overdamped motion of a particle in a double-well potential. The cubic map, however, possesses far richer dynamics as a function of the control parameter. In this contribution, we first study the dynamics of the cubic map with additive noise in analytical and numerical detail and compare it with the corresponding nonlinear Langevin equation. Considering two globally coupled cubic maps with additive noise, we analyze their potentially correlated dynamics as a function of the noise strength.

DY 10.8 Tue 11:30 ZEU 160

1/f noise from nonlinear stochastic differential equations driven by Lévy noise. — •Rytis Kazakevičius and Julius Ruseckas — Institute of Theoretical Physics and Astronomy, Vilnius University, A. Gostauto 12, LT-01108 Vilnius, Lithuania

The Lévy process constitute the most general class of stable processes while the Gaussian process is their special case. The physical reason behind the Lévy non-Gaussian processes traces back to the nonhomogeneous structure of the environment, in particular, fractal or multifractal [1]. A class of nonlinear stochastic differential equations providing the power-law behavior of spectra, including $1/f$ noise, and the power-law distributions of the probability density has been proposed [2]. Usually such equations are driven by white Gaussian noise. We have generalized the nonlinear stochastic differential equations to be driven by Lévy noise instead of Gaussian noise. To preserve statistical properties of the generated signal we have changed the drift term in the equations. We have analyzed two cases when the signal is positive and when the signal can also be negative. In contrast to the equation with the Gaussian noise, the constant in the drift term is different in those two cases.

[1] T. Srokowski, Phys. Rev E **78**, 031135 (2008).

[2] B. Kaulakys, J. Ruseckas, V. Gontis and M. Alaburda, Physica A **365**, 217 (2006).

DY 10.9 Tue 11:45 ZEU 160

Spectra of delay-coupled heterogeneous noisy nonlinear oscillators — •Andrea Vüllings[1], Eckehard Schöll[1], and Benjamin Lindner[2,3] — [1]Institut für Theoretische Physik, TU Berlin — [2]Physics Department, Humboldt University Berlin — [3]Bernstein Center for Computational Neuroscience Berlin

We study the spectral statistics (power and cross-spectral densities) of a small number of noisy nonlinear oscillators and derive analytical approximations for these spectra. The individual oscillators are described by the normal form of a supercritical or subcritical Hopf bifurcation supplemented by Gaussian white noise. Oscillators can be distinguished from each other by their frequency, bifurcation parameter, and noise intensity. Extending previous results from the literature, we first calculate in linear response theory the power spectral density and response function of the single oscillator in both super- and subcritical parameter. For small heterogeneous groups of oscillators (N = 2 or 3), which are coupled by a delayed linear term, we use a linear response ansatz to derive approximations for the power and cross-spectral densities of the oscillators within this small network. Using the theory we relate the peaks in the spectra of the homogeneous system (identical oscillators) to periodic solutions of the deterministic (noiseless) system. For two delay-coupled subcritical Hopf oscillators, we show that the coupling can enhance the coherence resonance effect, which is known to occur for the single subcritical oscillator. In the case of heterogeneous oscillators, we find that the delay-induced characteristic profile of the spectra is conserved for moderate frequency detuning.

DY 10.10 Tue 12:00 ZEU 160

Modulation of noise effects in nonlinear systems by time-delayed feedback — •Paul Geffert[1], Wolfram Just[2], Eckehard Schöll[1], Andrea Vüllings[1], and Anna Zakharova[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Queen Mary, University of London, School of Mathematical Sciences, UK

We study noise-induced phenomena in nonlinear systems under the influence of stochastic forces and time delay, and show that they can be controlled by time-delayed feedback. In particular, we discuss coherence resonance and stochastic bifurcations in single and coupled systems described by a subcritical Hopf normal form. For the case of time delayed feedback, we derive the stationary probability distribution by means of a multiple scale perturbation expansion. By applying statistical linearization techniques, we obtain analytic expressions for the autocorrelation function of the delayed system.

DY 10.11 Tue 12:15 ZEU 160

Stochastic modelling of wind turbines' athmospheric interactions assuming a diffusion process — •Benjamin Wahl[1,2], Matthias Wächter[2], Ulrike Feudel[1], and Joachim Peinke[2] — [1]Institute for Chemistry and Biology of the Marine Environment, University of Oldenburg, Germany — [2]ForWind and Institute of Physics, University of Oldenburg, Germany

The Langevin analysis has been successfully applied on single wind turbines to model the conversion from wind speed to power output with respect to the underlying turbulent dynamics. This motivates us to investigate the dynamical relationship of these quantities when they mix up from two different turbines. Therefor, we have to consider additional degrees of freedom naturally arising by the fact that the quantities of interest are measured spatially different. On the one hand the wind direction is changing over time and on the other hand the time delay of wind which is traveling from turbine to turbine is distorted due to turbulence. The split of the dynamics into a deterministic and a stochastic part should reveal a relaxation process, which we assume to exist, for instance, between two power outputs.

DY 11: Microswimmers (joint session DY/ BP)

Time: Tuesday 9:30–12:30 Location: ZEU 146

DY 11.1 Tue 9:30 ZEU 146

Aftrican trypanosomes swim faster in small capillaries and heterogeneous environment — •Davod Alizadehrad and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Germany

Human African trypanosome (HAT), the causative agent of the deadly sleeping sickness in sub-Saharan Africa, is a protozoan or single- celled microorganism that propels itself with the help of a beating flagellum. Despite good recent progress [1], refined models and further numerical simulations are necessary to uncover the heavily debated propulsion mechanism of the trypanosome, in particular, how the flagellum is attached to the cell body.

In this study, to simulate the swimming trypanosome, we construct a refined elastic network model of trypanosome based on experimental data and combine it with the mesoscale simulation technique called multi-particle collision dynamics (MPCD) to model the fluid environment. We reproduce several key features of trypanosome motility. First, we simulate the swimming and rotation speed of the trypanosome and find excellent agreement with experiments [2]. Second, we show that confinement has profound effects on trypanosome locomotion. In narrow circular channels the swimming speed increases up to 6 times its bulk value. Finally, we demonstrate that randomly distributed obstacles in a fluid help the trypanosome to swim more efficient.

[1] S.B. Babu and H. Stark, New J. Phys. 14, 085012 (2012).

[2] N. Heddergott, et al., PLoS Pathog, 8, e1003023 (2012).

DY 11.2 Tue 9:45 ZEU 146

Energetic efficiency of ciliary propulsion — •Andrej Vilfan and Natan Osterman — J. Stefan Institute, Ljubljana, Slovenia

Energetic efficiency of swimming has long been considered a non-issue in microorganisms, but newer studies show that ciliates can use more than half of their energy for propulsion. To estimate how close the ciliates are to the theoretically optimal way of swimming we address

the following problems: i) we determine the optimal stroke of a cilium, ii) we determine the optimal beating pattern of a ciliated surface and iii) we calculate the optimal shape of a ciliated swimmer.

For a single cilium we define the efficiency in a scale-invariant way and show that the optimal stroke consists of a working stroke with a stretched cilium and a recovery stroke where the cilium bends and moves closer to the surface. When optimizing an array of cilia we additionally show that metachronal waves improve the efficiency and that the optimal efficiency is achieved for antiplectic waves. The resulting beating patterns, as well as the optimal ciliary density, show remarkable similarity with those observed in ciliated microorganisms. In order to optimize the shape of the whole swimmer we use a simplified description where we replace the ciliated layer with a surface slip velocity. The optimal shapes again resemble those of different ciliates. If we combine the results of our optimization with experimental efficiency estimates we can show that Paramecium has a propulsion efficiency that is within a factor of 2 of the theoretical optimum.

[1] N. Osterman and A. Vilfan, PNAS 108, 15727 (2011) [2] A. Vilfan, Phys. Rev. Lett. 109, 128105 (2012)

DY 11.3 Tue 10:00 ZEU 146

Hydrodynamics of spherical microswimmers in a quasi-2D geometry — •Andreas Zöttl and Holger Stark — TU Berlin

Microorganisms like bacteria, sperm cells or algae live in aqueous environments and their motion is therefore governed by low-Reynolds-number hydrodynamics, but also influenced by thermal and biological noise. Experiments with artificial microswimmers, which are used to study collective motion of self-driven particles out of equilibrium, are often performed in a quasi-2D geometry or in thin films, where dynamic clustering and motility-induced phase separation is observed.

Motivated by recent experiments of active colloids and emulsion droplets in confinement, we also study the collective motion of spherical squirmers moving in a quasi-2D geometry by means of multi-particle collision dynamics. Hydrodynamic near-field interactions between swimmers lead to hydrodynamic rotational diffusion, while hydrodynamic interactions between the channel walls and swimmers strongly influence the preferred swimmer orientations and therefore the formation of hexagonal clusters. Neutral squirmers in particular separate into a gas-like and a crystalline phase which we characterize by a structural order parameter. Varying the density of the swimmers from low to high area fraction results in a steep increase of the order parameter at the critical density, accompanied by strong fluctuations indicating a non-equilibrium phase transition which is absent for strong pullers and pushers.

DY 11.4 Tue 10:15 ZEU 146

Optimization of bead-spring micro-swimmers and study of dense swimmer solutions — •Jayant Pande[1,2] and Ana-Sunčana Smith[1,2] — [1]Institute for Theoretical Physics, Friedrich-Alexander University, Erlangen, Germany — [2]EAM: Cluster of Excellence, Friedrich-Alexander University, Erlangen, Germany

With the increasing need to understand and predict the locomotion of natural organisms and machines at the micro-scale, the theoretical modelling of micro-swimmers has become an important field of study. Contributing to its development, we present analytical results on the geometric and kinematic optimization of three-ellipsoid microswimmers, based on the three-sphere model of Najafi and Golestanian. Assuming a sinusoidal driving protocol, we identify different drag-related regimes and determine the exact shapes which maximise the swimming velocity and efficiency in each regime. Conditions on the optimal forcing parameters as well as the push/pull nature of the swimmer are elucidated. The analytical work is supported by simulations using an in-house framework based on the lattice-Boltzmann method. Its versatility and massively-parallel capabilities allow us to explore near-field effects as well as those arising from asymmetry in the swimmer design. We show that these effects, while inaccessible to an exact theoretical treatment, are nevertheless amenable to an approximate description. In the last part of our contribution, we employ our simulation system to study large populations of passive and active particles in fluids. For different concentrations, we observe previously-known effects as well as departures from theory.

DY 11.5 Tue 10:30 ZEU 146

Statistical properties of tracer positions, sedimenting in an active fluid — •Thomas John, Matthias Mussler, and Christian Wagner — Experimentalphysik, Universität des Saarlandes

Fluid dynamics on μm scale at velocities in μm/s is characterized by very low Reynolds numbers. Therefore no turbulent behavior and characteristics is expected. Nevertheless, a spatial-temporal random flow field can be present in a media if the fluid contains a lot of active, irregular moving micro-swimmers. We consider trajectories of passive sedimenting beads in such fluids. This trajectories are strongly influenced from the random flow field if the passive particle (tracer) diameter comparable or less then the diameter of the micro-swimmers. We measured such trajectories in suspensions of the green alga chlamydomonas reinhardtii. The alga has two flagella, a diameter of 10 μm and swims as a puller with 50 μm/s. We extract statistical properties of the passive bead positions, e.g. the mean square displacement or the probability density function. Our results are compared with the Brownian motion characteristics of sedimenting particles in very dilute systems and the known non-Brownian characteristics in passive sedimenting particles at higher volume concentrations where the hydrodynamic interactions becomes important.

DY 11.6 Tue 10:45 ZEU 146

Propulsion of droplets by rigidly tethered traction forces — •P. Sekhar Burada, Reiner Kree, and Annette Zippelius — Institute for Theoretical Physics, University of Göttingen, Germany

We study the dynamics of an active droplet, with both translational- and rotational degrees of freedom. A field of interfacial traction forces, which is time independent in a body-fixed reference frame drives the system. Using the general solution of the Stokes equation, with the appropriate boundary conditions, we are able to calculate the hydrodynamic flow pattern both inside and outside of the droplet. Also, using force- and torque balance conditions the translational- and rotational velocities of the droplet are calculated. We derive the conditions, in terms of mode amplitudes of the traction force, which need to be satisfied in order to preserve the shape of the droplet.

15 min break

DY 11.7 Tue 11:15 ZEU 146

Transport powered by bacterial turbulence — •Andreas Kaiser[1], Anton Peshkov[2], Andrey Sokolov[3], Borge ten Hagen[1], Hartmut Löwen[1], and Igor S. Aranson[3] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf — [2]Service de Physique de l'Etat Condensé, Gif-sur-Yvette — [3]Materials Science Division, Argonne National Laboratory

We show that turbulence in a bacterial bath can be exploited to power and steer directed transport of mesoscopic carriers through the suspension. In our experiments and simulations, a microwedge-like "bulldozer" is exposed to a bacterial bath of varied concentration and obtains a maximal transport speed in the turbulent state of the bacterial suspension.

DY 11.8 Tue 11:30 ZEU 146

Cell body rocking is dominant mechanism for flagellar synchronization in a swimming alga — Veikko Geyer[1], Frank Julicher[2], Jonathon Howard[1], and •Benjamin Friedrich[2] — [1]Max Planck Institute for Cell Biology and Genetics — [2]Max Planck Institute for the Physics of Complex Systems

The eukaryotic flagellum is a best-seller of nature: These slender cell appendages propel sperm and many other microswimmers, including disease-causing protists. In mammalian airways and the oviduct, collections of flagella beat in synchrony to pump fluids efficiently. Here, we report on theory and experiment that elucidate a mechanism of flagellar synchronization in the model organism *Chlamydomonas*, a green algal cell that swims with two flagella like a breaststroke swimmer. Our analysis shows how synchronization arises by a coupling of swimming and flagellar beating and characterizes an exemplary force-velocity relationship of the flagellar beat. Any perturbation from the synchronized state causes the cell body to rock, which changes the hydrodynamic friction forces acting on the flagella and thus their speed, which restores their synchronization.

Geyer *et al.*: Proc. Natl. Acad. Sci. U.S.A. **110**, 2013.

DY 11.9 Tue 11:45 ZEU 146

Direct Measurements of Active Flagellar Fluctuations — •Benjamin Friedrich[1], Rui Ma[2], Gary Klindt[1], Frank Julicher[1], and Ingmar Riedel[3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Institute for Advanced Study, Tsinghua University, Beijing, China — [3]Department of Bioengineering, Stanford University, Stanford, CA, USA

The eukaryotic flagellum beats regularly, driven by the oscillatory dynamics of molecular motors, to propel cells and pump fluids. Small, but perceivable fluctuations in the beat of individual flagella have physiological implications for synchronization in collections of flagella as well as for hydrodynamic interactions between flagellated swimmers. Here, we characterize phase diffusion and amplitude fluctuations of sperm flagellar beat patterns. We employ shape mode analysis and limit cycle reconstruction for a low-dimensional representation of flagellar bending waves. We find that flagellar fluctuations are dominantly of active origin. Using a minimal model of collective motor oscillations, we demonstrate how active fluctuations can naturally arise from the stochastic dynamics of individual motors.

DY 11.10 Tue 12:00 ZEU 146

Synchronization of rigid microrotors by time-dependent hydrodynamic interactions — •Mario Theers and Roland Winkler — Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Juelich, D-52425 Juelich, Germany

The synchronized beating of flagella is fundamental for the coordinated motion of microswimmers such as spermatozoa, bacteria, protozoa, or algae. It is a longstanding conjecture that this microscopic synchronization could be induced by hydrodynamic interactions. However, synchronization is not easily achieved for low Reynolds-number fluids, which are described by Stokes equations. The presence of kinematic reversibility combined with swimmer symmetries may prevent synchronization.

We provide an extension of previous low-Reynolds number studies by analyzing the linearized, time-dependent Navier-Stokes equations instead of the usually adopted Stokes equations. As a model system, we investigate the emergent dynamical behavior of hydrodynamically coupled microrotors and demonstrate that time-dependent hydrodynamic interactions inevitably lead to synchronization of their rotational motion, which is not achieved on the basis of Stokes equations. We show that the system can be described by coupled nonlinear integro-differential equations and derive analytical results for the the phase difference. Additionally, results are compared to mesoscale hydrodynamic simulations. Our studies provide a deeper insight into the nature of hydrodynamic interactions between microswimmers.

DY 11.11 Tue 12:15 ZEU 146

A close look at the tumbling of bacteria — •Tapan Chandra Adhyapak and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin

Peritrichous bacteria such as Escherichia coli propel themselves by using multiple flagella, each rotated at the base by a rotary motor. Hydrodynamic interactions together with an intricate balance of elasticity of the flagella cause them to synchronize and form a single bundle leading to propulsion in a straight line. Such straight runs of a bacterium frequently terminate at relatively short lived tumbling events during which one or more of the flagella leave the bundle disrupting uniform motion and causing the bacterium to change its course. In addition to hydrodynamic interactions and elasticity, rotation-induced polymorphic transitions between different flagellar states [1] is observed to play an important role in re-orientating the bacterium. The detailed process however is complex and very little understood. We investigate the tumbling strategy of an E. Coli modelling its propulsion using an extended continuum theory of elasticity in presence of hydrodynamic interactions. We examine, in particular, the effect of rotation-induced polymorphic transitions of flagella during such processes.

[1] R. Vogel and H. Stark, Phys. Rev. Lett. **110**, 158104 (2013).

DY 12: Complex Fluids and Soft Matter (joint session DY/ CPP/ BP)

Time: Tuesday 9:30–11:30 Location: ZEU 118

DY 12.1 Tue 9:30 ZEU 118

Microrheology of shear thinning solutions — •Juan Ruben Gomez-Solano[1,2] and Clemens Bechinger[1,2] — [1]Universitaet Stuttgart, 2. Physikalisches Institut, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, 70569 Stuttgart, Germany

Colloidal probes embedded in complex fluids have been extensively employed to investigate their rheological response to small stress. However, this approach is not evident for fluids subjected to large stresses, where a variety of non-Newtonian behaviors can occur. One example of such systems are semi-dilute micellar solutions, which consist of surfactant molecules forming worm-like micelles entangled in aqueous solution. In this work, we study the motion of a colloidal probe dragged by an optical trap through a semi-dilute micellar solution of cetylpyridinium chloride. The motion of the probe creates a shear strain, which depends linearly on its mean velocity v. We measure the effective viscous drag on the probe and the fluctuations of its position as a function of v. We find that at small v, the system can be characterized by a constant viscosity, whereas the position fluctuations are statistically the same as in thermal equilibrium. However, above a certain value, the viscosity decreases as a function of v. The fluctuations of the particle position are also affected in the shear-thinning regime, and their power spectral density increases with increasing v. We find that the transition between both regimes typically occurs when the shear rate exceeds the inverse relaxation time of the entangled micelles.

DY 12.2 Tue 9:45 ZEU 118

Shear driven instabilities in anisotropic colloidal mixtures — •Rodrigo Lugo-Frias and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In recent years much attention has been paid in understanding the orientational order of anisotropic hard bodies in the presence of steady shear flow [1,2]. On the other hand, sheared systems of binary mixtures of hard disc and rodlike particles have also been examined [3].

We focus in the nonequilibrium dynamics of a binary mixture of rodlike nematic polymers under shear flow. To do so, we derive from density functional theory (DFT) a mesoscopic free energy in terms of the alignment tensor for each component. We proceed to investigate their dynamical behavior using the well known mesoscopic Doi–Hess theory, which lead to a set of nonlinear differential equations [4,5,6]. Finally, we examine the total alignment of each component and its dependencies with the physical properties of the system.

[1] S. H. L. Klapp and S. Hess, Phys. Rev. E **81**, 051711 (2010).
[2] D. Strehober, H. Engel and S. H. L. Klapp, Phys. Rev. E **88**, 012505 (2013).
[3] F. Tardani, L. Gentile, G. A. Ranieri and C. La Mesa, J. Phys. Chem. C, **117**, 8556 (2013).
[4] S. Hess, Z.Naturforsch. A **31a**, 1034 (1976).
[5] M. Doi, J.Polym. Sci., Polym. Phys. Ed. **19**, 229 (1981).
[6] S. Hess and M. Kröger, J.Phys.: Cond. Matter, **16**, S3835 (2004).

DY 12.3 Tue 10:00 ZEU 118

Friction of Colloidal Crystals on Commensurate and Incommensurate Substrates — •Aleksandar Mijailović and Michael Schmiedeberg — Theoretische Physik 2, Heinrich-Heine Universität, Düsseldorf, Germany

Among the fascinating properties of quasicrystals - structures that possess long range order but no translational symmetry - is the very low friction that was observed when a periodic crystal is moved over the surface of a quasicrystal [1]. Here we want to explore whether there are geometrical reasons for the small friction.

Using Brownian Dynamics simulations, the friction properties of 3D colloidal fcc-crystals on substrates with different geometries are studied. We measure the friction as a function of the drag force applied on the crystal, from which the friction coefficient is extracted. We repeat this analysis for commensurate, incommensurate perodic, and quasicrystalline substrates and investigate the effect of incommensurability as well as aperiodicity.

The (charged) colloidal particles are interacting via the Asakura-Oosawa Model, i.e., a superposition of the screened-Coulomb potential and an attractive term, which is due to the presence of non-adsorbing polymers (not treated explicitly). Finally, our results are compared to the 2D case (cf., e.g., [2].

1. J. Y. Park *et al.*, *Science* **309**, 1354 (2005).
2. T. Bohlein *et al.*, *Nat. Mat.* **11**, 126 (2012).

DY 12.4 Tue 10:15 ZEU 118

Complex dynamics of a bilamellar vesicle as a simple model for leukocytes — •Badr Kaoui — Theoretical Physics I, University of Bayreuth, 95440 Bayreuth, Germany — Department of Applied Physics, Eindhoven University of Technology, P. O. Box 513, 5600 MB Eindhoven, The Netherlands

The influence of the internal structure of a biological cell (e.g., a leukocyte) on its dynamics and rheology is not yet fully understood. By using 2D numerical simulations of a bilamellar vesicle (BLV) consisting of two vesicles as a cell model, we find that increasing the size of the inner vesicle (mimicking the nucleus) triggers a tank-treading-to-tumbling transition. A new dynamical state is observed, the undulating motion: the BLV inclination with respect to the imposed flow oscillates while the outer vesicle develops rotating lobes. The BLV exhibits a non-Newtonian behavior with a time-dependent apparent viscosity during its unsteady motion. Depending on its inclination and on its inner vesicle dynamical state, the BLV behaves like a solid or a liquid [Badr Kaoui, Timm Krüger and Jens Harting, Soft Matter 9, 8057 (2013)].

15 min break

DY 12.5 Tue 10:45 ZEU 118

Random Organization and Jamming within a unifying model system — •Lars Milz[1] and Michael Schmiedeberg[2] — [1]Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Institut für Theoretische Physik 2: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40204 Düsseldorf, Germany

We show that both random organization and jamming occur within the same model packing problem despite the obvious differences between these two transitions: The random organization transition describes the change from reversible to irreversible dynamics in a non-equilibrium system and the athermal jamming transition occurs when particles can no longer avoid overlaps if quenched from infinite to zero temperature.

In our unifying model system the particles are initially randomly distributed and then displaced in each step if they overlap. For random displacements we obtain a random organization transition while jamming occurs in case of deterministic shifts. For the random organization transition, we also determine the critical exponents. For the jamming transition we observe a divergence of the relaxation time of our method.

Within our model system, random organization and jamming are opposite limits of random sphere packings. In future, we want to study intermediate packing problems or mixtures or random organization and jamming that probably correspond to other equilibrium or non-equilibrium transitions.

DY 12.6 Tue 11:00 ZEU 118

Foam morphology, frustration and topological defects in a Negatively curved Hele-Shaw geometry — •Adil Mughal, Myfanwy Evans, and Gerd Schröder-Turk — Institut fur Theoretische Physik, Friedrich-Alexander Universitat Erlangen-Nurnberg, Staudtstr. 7, D-91058 Erlangen, Germany

We present preliminary simulations of foams and single bubbles confined in a narrow gap between parallel surfaces. Unlike previous work, in which the bounding surfaces are flat (the so called Hele-Shaw geometry), we consider surfaces with non-vanishing Gaussian curvature.

We demonstrate that the curvature of the bounding surfaces induce a geometric frustration in the preferred order of the foam. This frustration can be relieved by the introduction of topological defects (disclinations, dislocations and complex scar arrangements). We give a detailed analysis of these defects for foams confined in curved Hele-Shaw cells and compare our results with exotic honeycombs, built by bees on surfaces of varying Gaussian curvature.

Our simulations, while encompassing surfaces of constant Gaussian curvature (such as the sphere and the cylinder), focus on surfaces with negative Gaussian curvature and in particular triply periodic minimal surfaces (such as the Schwarz P-surface and the Schoen's Gyroid surface). We use the results from a sphere-packing algorithm to generate a Voronoi partition that forms the basis of a Surface Evolver simulation, which yields a realistic foam morphology.

DY 12.7 Tue 11:15 ZEU 118

Molecular simulation methods to compute interfacial free energies — •Ronald Benjamin and Juergen Horbach — Theoretical Physics II, Heinrich-Heine Universitaet, 40225 Duesseldorf, Germany

Knowledge of interfacial free energies are crucial to understanding physical phenomena such as wetting and nucleation. In this talk we discuss several ways to extract this quantity for wall-liquid and wall-crystal interfaces. Chiefly, we discuss a new thermodynamic integration scheme developed to determine the interfacial free energy and compare it to a non-equilibrium work method and a Gibb's-Duhem type of approach known as "Gibb's-Cahn integration".

We also extended our thermodynamic integration scheme to obtain the excess free energy of a supercooled liquid in contact with amorphous walls having the same structure as the liquid. Our results shed new light on the thermodynamic behavior of supercooled liquids and help explain their slowing down in the presence of such rough walls.

DY 13: Poster - Glasses / Stat. Phys. Bio. / Networks (joint session DY/BP/CPP/SOE)

In this poster session there are contribution from
- Focus Session: Slow Dynamics in Glasses and Granular Matter
- Focus Session: Feedback Control - Soft and Hard Matter
- Glasses
- Statistical Physics in Biological Systems
- Networks - Statistics and Dynamics

Time: Tuesday 9:30–12:30 Location: P1

DY 13.1 Tue 9:30 P1

Investigation of the behavior of binary mixtures upon variation of the dynamic asymmetry — •Marie-Luise Braatz[1], Sebastian Schramm[1], Thomas Blochowicz[1], Bernd Stühn[1], and Bernhard Frick[2] — [1]Experimental Condensed Matter Physics, TU Darmstadt, Germany — [2]Institut Laue Langevin, Grenoble, France

We study dynamically asymmetric binary mixtures comprised of polystyrene and the small molecule methyl tetrahydrofuran (MTHF). The blends are fully miscible on supercooling but still exhibit two glass transition temperatures. Between these two temperatures MTHF relaxes in a matrix of polystyrene, showing the signature of geometrical confinement on the nanoscale in its dynamic properties. Among the interesting characteristics observed, is a transition from fragile to strong behavior of the time constants and in some cases features of a type-A glass transition are found.

We study the behavior of these characteristics upon varying the molecular weight and thereby the dynamic asymmetry of the mixture as well as the concentration of the small molecules. Dielectric spectroscopy, depolarized dynamic light scattering and quasielastic neutron scattering are combined to cover a dynamic range of 1ps to 1000s.

Our results are compared to theoretical predictions that expect fragile-strong transitions and type-A glass transitions to be most pronounced at low concentrations of the small molecules and large dynamic asymmetries.

DY 13.2 Tue 9:30 P1

Mesoscale modeling of aeolian sand transport — •Anne Meiwald, Marc Lämmel, and Klaus Kroy — Institut für Theoretische Physik, Leipzig, Germany

Aeolian transport of sand is one of the most important geological pro-

cesses on Earth and other rocky planets, creating a wide range of self-organised dynamic structures, like ripples or sand dunes. To make the complex grain physics more amenable to analytical studies, it was proposed to coarse-grain the ensemble of grain trajectories by two types representing low-energetic reptating grains and high-energetic saltating grains [1]. We recently showed that our analytically tractable and numerically efficient continuum model reliably reproduces sand flux measurements obtained in various wind tunnel experiments [2].

Here, we scrutiny the potential of our approach to predict important grain-scale properties and find remarkable agreement with various experimental data. We also speculate about the reason for the success of the coarse-grained description, even in comparison to more detailed numerical models, despite its allegedly unfaithful representation of some of the grain-scale details [3]. Finally we conclude that the two-species continuum approach provides an appropriate starting point for analytical and efficient numerical modelling of seemingly complex aeolian saltation process and the structures it creates.

[1] Bagnold, *The physics of blown sand and desert dunes.* Dover Publ. (2005).
[2] Lämmel, Rings, and Kroy, New J. Phys. 14, 093037 (2012).
[3] Kok, and Renno, J. Geophys. Res. 114, D17204 (2009).

DY 13.3 Tue 9:30 P1

Railway buckling safety: From Theory to application — •János Török[1], László Halma[2], and István Fejér[2] — [1]Department of Theoretical Physics,Budapest University of Technology and Economics, H-1111 Budapest, Hungary — [2]Vasútépítök Kft, H-9023 Györ, Csaba utca 9

Using numerical simulation and mesoscopic theory we show that in granular materials the effective friction coefficient at walls depends heavily on the wall roughness. We show that it can be used in real application. In continuous welded rails the standard railbed in small radius curves are not able to resist the radial load arising from temperature and train movement. Today many different and expensive methods are used to tackle this problem. We show that by making the bottom of the sleepers rough we can increase the buckling safety of the track.

DY 13.4 Tue 9:30 P1

Continuum Mechanics Simulations of Nonlinear Deformation of Viscoplastic Solids — •Heliana Cardenas[1] and Thomas Voigtmann[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany — [2]Zukunftskolleg und Fachbereich Physik, Universität Konstanz, Konstanz, Germany

When amorphous solids are formed by solidification of dense liquids slow intrinsic relaxation plays a determining role on describing their behavior. Systems like this can be perturbed by external mechanical fields driving it to a non-equilibrium regime following then non-linear deformation laws. The mode-coupling theory of the glass transition (MCT) has been extended to describe the interplay between strong external forces and slow relaxation.

A non-linear extension of the Maxwell model of viscoelastic fluids is proposed. This model takes into account the relaxation time dependence on the shear rate and thereby mimics microscopic processes identified by MCT. Combining this constitutive equation with the Navier-Stokes equations we can describe the evolution of macroscopic flows. Attention will be focused on shear-thinning fluids where the fluid's viscosity decreases with an increasing rate of shear stress.

To solve non-linear integro-differential equations finite element modeling (FEM) is used through a computational fluid dynamics tool. The effect of different relaxation times for a pressure driven flow is studied by analyzing velocity profiles, among other measurable quantities.

DY 13.5 Tue 9:30 P1

Mechanical Properties of Sheared Wet Granular Piles — •Somnath Karmakar[1], Marc Schaber[1], Anna-Lena Hippler[1], Martin Brinkmann[2], Mario Scheel[3], Marco Di Michiel[3], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]MPI for Dynamics and Self-Organization, Göttingen, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France

Adding small amount of wetting fluid to dry granulates typically leads to the granular stiffness which arises due the formation of minute liquid contacts between individual granules by the virtue of capillary forces. We experimentally study the mechanical properties of wet granulates, composed of monodisperse spherical glass or basalt beads. The glass microspheres are almost perfectly wetted by water whereas the basalt microspheres have a rather large contact angles with water. The different wettability causes a difference in the shape and volume distribution of the appeared liquid morphologies. We have investigated the shear strength, measured under cyclic shear deformation for various system parameters like liquid content, shear rate and absolute pressure. At large absolute pressures, the associated energy dissipation of a sheared wet granulate is considerably smaller than that of a completely dry bead assembly; where the wetting fluid might act as a 'liquid lubricant' by lowering the wet bead pile's shear stiffness. With time resolved X-ray microtomography, we could shed some light on the underlying microscopic mechanisms of the sheared wet granulates.

DY 13.6 Tue 9:30 P1

Stability of Barchan Dune Fields — •Sven Auschra, Marc Lämmel, and Klaus Kroy — Institut für theoretische Physik, Leipzig, Germany

Crescent-shaped barchan dunes are among the most impressive structures observed in arid regions on Earth and Mars. Although they are isolated from nearby dunes by bedrock, models suggests that truly isolated barchans would be unstable with respect to their mass balance [1]. This suggests that some sort of interactions between the dunes in a dune field give rise to some size stabilization resulting in the empirically observed uniform size distribution along the dune field [2, 3].

To uncover the underlying mechanism, we perform a mass stability analysis for a pair of consecutive dunes in a barchan field. Sand supplied from the horn of the windward dune to its downwind neighbor initiates a complex response of its shape and mass. Based on a dimensionally reduced description justified by a closeby shape attractor, a one-dimensional fixed-point equation for the mass balance of the downwind dune is derived and analyzed for stable solutions.

[1] Fischer, Cates and Kroy, Phys. Rev. E 77, 031302, 2008.
[2] Hersen, Andersen, Elbelrhiti, Andreotti, Claudin and Douady, Phys. Rev. E 69, 011304, 2004.
[3] Duran, Schwämmle, Lind and Herrmann, Nonlin. Processes Geophys. 69, 455-467, 2001.

DY 13.7 Tue 9:30 P1

Ab-inito MD parameter estimation for Na diffusion in glasses — •Lars Winterfeld and Erich Runge — Institut für Physik, TU Ilmenau, 98693 Ilmenau

Molecular dynamics (MD) simulation provide a scalable method for the investigation of disordered systems like glasses. However, there is no generally accepted method for the determination of the MD model parameters. We present a new first-principle approach that allow us to self-consistently obtain such parameters by sampling an ensemble of representative configurations. We use MD to create these configurations and run ab-initio DFT calculations as basis for the subsequent fitting procedure. Results of this approach are compared for $(Na_2O)_x - SiO_2$ glass systems with those from the literature.

DY 13.8 Tue 9:30 P1

Non-universal dielectric properties of glasses at very low temperatures — •Annina Luck, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, INF227, D-69120 Heidelberg

The universal behaviour of amorphous solids at low temperatures, governed by two level tunneling systems, has long been a generally accepted fact. In the last years, however, measurements of dielectric two-pulse polarization echoes have revealed that nuclear electric quadrupole moments involved in atomic tunneling sytems can cause specific material-dependent effects in magnetic fields.

To study the possible influence of nuclear electric quadrupoles connected with atomic tunneling systems on the low frequency dielectric properties of glasses down to a temperature of 10 mK, we measured the multicomponent glass N-KZFS11, which contains 25 mass percent of tantalum oxide and a glass containing a similar amount of holmium oxide. As ^{181}Ta and ^{165}Ho carry very large nuclear electric quadrupole moments,these glasses seem to be ideal candidates to determine the influence of nuclear electric quadrupole moments on the physical properties of glasses at low temperatures.

Our measurements not only show a non-universal dieletric behaviour in the two glasses, but also differ significantly from various predictions of the standard tunneling model. We discuss these new findings in the framework of the tunneling model.

DY 13.9 Tue 9:30 P1

Understanding the properties of two dimensional silica systems — •ProjeshKumar Roy[1] and Andreas Heuer[2] — [1]Graduate school of chemistry, University of Muenster — [2]Institute of physical chemistry, University of Muenster

Recently, STEM and SPM studies were performed by Lichtenstein et al, [1] in a virtually two dimensional silica bilayer; which was grown by depositing vaporised Si atoms on a [Ru(0001)] metal surface in an oxygen atmosphere. Silica bilayers were generated, which could be either amorphous or crystalline, depending on the preparation conditions. Under specific conditions even both states could be generated in the same layer, including a short-range transition between them. Remarkably, even in the amorphous case both layers were virtually identical. Due to the atomic resolution the ring statistics in the amorphous structure could be characterized in detail.

We report about computer simulations which have the aim to reproduce the properties of two-dimensional silica layers and, consequently, obtain an improved microscopic understanding of this system. In particular we want to learn, under which conditions crystalline and amorphous structures can be generated, respectively. For this purpose, an appropriate silica potential has to be developed which can be used in the two-dimensional case and is able to generate the observed structural features.

[1] Lichtenstein L; Heyde M; Freund H.J.; J. Phys. Chem. C 2012, 116, 20426.

DY 13.10 Tue 9:30 P1

Understanding the energy landscape of a simple water model — •Katharina Ferling and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster

Liquid water plays an important role not only in our everyday life but also in simulations and experiments where it serves as a solute with many applications. The understanding of the water behaviour, including its anomalies, can play an important role in improving the description of water. Here the emphasis lies on the property of building H-bonds which is believed to be one major factor for many anomalies such as the density change or the liquid-liquid phase transition at low temperatures. For the present investigation a simple model has been chosen which focuses on the distinction between a close-packed and an open structure. The one dimensional model - which was first introduced by Ben-Naim [1,2] - has now been extended with additional long range interactions in the underlying potential to get rid of the mean-field character of that model. First, simulations are performed in the NPT-ensemble with the aim to show water-like behaviour such as a high-density liquid and low-density liquid (HDL-LDL) transition. Second, from simulations in the NVT-ensemble for different volumes (lengths, resp.) a closer understanding of the possible anomalies can be reached, related to properties of the underlying potential energy landscape.

[1] Arieh Ben-Naim, J. Chem. Phys. 128, 024505 (2008)
[2] Lotta Heckmann and Barbara Drossel, J. Chem. Phys. 137, 064503 (2012)

DY 13.11 Tue 9:30 P1

Compressed exponential decays in correlation experiments: The influence of temperature gradients and convection — •Jan Gabriel, Thomas Blochowicz, and Bernd Stühn — Institut für Festkörperphysik, Darmstadt

In a wide range of correlation experiments using laser light or partially coherent X-rays so called compressed exponential correlation functions were reported [1] i.e. decays $c(\tau) \propto \exp(-(t/\tau)^{\beta})$ with $\beta > 1$. The source of this phenomenon is still a point of discussion. For example for colloidal particles in supercooled liquid [2] it is claimed that near T_g hyperdiffusive behavior appears, which leads to compressed correlation functions.

We performed multispeckle-dynamic light scattering experiments in a temperature range from 230 K to 300 K with a sCMOS camera in a system of Polystyrene spheres in supercooled propanediol. At low temperatures compressed exponential decays are observed. At the same time, however, the speckle pattern shows indication for convection in the sample due to a slight temperature gradient, across the sample cuvette mounted on a cold finger cryostat. These effects increase with decreasing temperature and after a temperature jump and can be corrected for by assuming convective flow at constant velocity. Such corrections reduce or remove compressed exponential behavior.

[1] A Madsen, R. L. Leheny, H. Guo, M Sprun and Orsolyal, New J. Phys., **12**, 055001 (2010)
[2] C. Caronna, Y. Chushkin, A. Madasen and A. Cupane, Phys. Rev. Lett., **100**, 055702 (2008)

DY 13.12 Tue 9:30 P1

Temperature and pressure dependence of the supramolecular structure of 2-ehyl-1-hexanol and 4-methyl-3-heptanol — •Thomas Büning[1], Christian Sternemann[1], Catalin Gainaru[2], Michael Paulus[1], Kolja Mende[1], Florian Wirkert[1], Irena Kiesel[1], Johannes Möller[1], Julia Nase[1], Stefan Bauer[2], Roland Böhmer[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund — [2]Fakultät Physik/E3, Technische Universität Dortmund, D-44221 Dortmund

Hydrogen bonds are essential for structure and dynamics of e.g. alcohols, aqueous solutions and water. Due to their low tendency to crystallization and large variability in molecular configuration, monohydroxy alcohols are a typical system that is studied to learn about the impact of hydrogen-bonding on molecular liquids. Because of the hydrogen bonds alcohols form supramolecular structures in the liquid phase. Here, the molecular arrangements of monohydroxy alcohols such as 2-ethyl-1-hexanol (2E1H) and 4-methyl-3-heptanol (4M3H) strongly depend on the position of the OH group within the molecule. Based on dielectric spectroscopy molecular arrangements in chain-like (2E1H) and, ring-like (4M3H) structures have been proposed. We present an x-ray diffraction study of 2E1H and 4M3H, providing new information regarding the supramolecular structure in pressure up to 4 kbar and temperature down to -110 °C.

DY 13.13 Tue 9:30 P1

Molecular Order and Dynamics of Nanometric Thin Layers of Poly(styrene-b-1,4-isoprene) Diblock Copolymers — •Wycliffe K. Kipnusu[1], Mahdy M. Elmahdy[1], Martin Tress[1], Emmanuel U. Mapesa[1], Detlef-M. Smilgies[2], Jianqi Zhang[3], Christine M. Papadakis[3], and Friedrich Kremer[1] — [1]Institute of Experimental physics I, Linnstr.5, 04103, Leipzig — [2]CHESS, Wilson Laboratory, Cornell University, Ithaca, NY 14853, USA — [3]Technische Universität München, Physik-Department, James-Franck-Straße 1, 85748 Garching, Germany

Order and dynamics of poly(styrene-block-1,4-isoprene), P(S-b-I) diblock copolymers in nanometer thin layers with different isoprene volume fraction (fPI) and identical molecular weight of the styrene blocks are studied by a combination of Grazing-Incidence Small-Angle X-ray Scattering (GISAXS), Atomic Force Microscopy (AFM) and Broadband Dielectric Spectroscopy (BDS). GISAXS and AFM reveal randomly oriented lamellar structures in the films and a parallel orientation at the top surface, respectively. Using BDS, three well separated relaxation processes are detected, (i) and (ii) the dynamic glass transitions (segmental mode) in the styrene and isoprene blocks respectively and (iii) the normal mode relaxation representing fluctuations of the isoprene chain as a whole or parts of it. While the two former do not show any thickness dependence in their spectral positions, the latter becomes faster with decreasing sample thickness. This reflects the difference in the length-scale on which the molecular fluctuations take place.

DY 13.14 Tue 9:30 P1

Intra- and inter-molecular dynamics in the course of vitrification in organic glasses — Ludwig Popp, Benjamin Suttner, •Wilhelm Kossak, and Friedrich Kremer — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik I, Linnestr. 5, 04103 Leipzig

FTIR and BDS are utilized to study the vitrification of various well known glass formers in a wide temperature range around the calorimetric glass transition temperature, Tg. Measurements on Propylene glycol, Glycerol, Salol, Benzophenone, Sorbitol, Xylitol, etc. are compared and the sub-molecluar specificity of the different moieties in their contribution to thermally activated processes including the dynamic glass transition are discussed. By that the necessity of atomistic models of the glass transition beyond coarse grained models is revealed.

DY 13.15 Tue 9:30 P1

The potential energy landscape of sheared glass-forming systems — •Markus Blank-Burian and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster, Deutschland

We performed molecular dynamics simulations of small supercooled binary Lennard-Jones mixtures ($65 <= N <= 1040$) under a con-

stant shear rate. The shearing is achieved by applying Lees-Edwards periodic boundary conditions to the system. The potential energy landscape (PEL) is most informative for small systems. However, we also study the influence of finite size effects on our results.

In previous work, it was shown, that the finite size effects in unsheared systems is quite small for thermodynamic observables and for the diffusivity. The dynamics of these systems can be described by a continous time random walk (CTRW) between minima in the potential energy landscape. Our focus now lies on comparing these results with the constantly sheared system.

In the sheared system, we test for finite size effects in general properties like the velocity profile or the shear viscosity. Since the potential energy landscape is now time-dependent, we use affine transformations to understand the temporal evolution of its minima. With this insight, we can use the same continuous time random walk analysis as with the unsheared system.

DY 13.16 Tue 9:30 P1

Self-stabilizing Learning Rules in Neural Models driven by Objective Functions — •Rodrigo Echeveste and Claudius Gros — Institut für Theoretische Physik, Johann Wolfgang Goethe Universität, Max-von-Laue-Str. 1, Frankfurt am Main, Germany

In the present work, learning rules for a neuronal model are derived from two objective functions. On the one hand, the neuron's firing bias is adjusted by minimizing the Kullback-Leibler divergence with respect to an exponential output distribution. On the other hand, learning rules for the synaptic weights are obtained by minimizing a Fisher information that measures the sensitivity of the input distribution with respect to the growth of the synaptic weights. In this way, we obtain rules that both account for Hebbian/anti-Hebbian learning and stabilize the system to avoid unbounded weight growth. As a by-product of the derivation, a sliding threshold, similar to the one found in BCM models, is obtained for the learning rules.

As a first application of these rules, the single neuron case is studied in the context of principal component analysis and linear discrimination. We observe that the weight vector aligns to the principal component when the input distribution has a single direction of maximal variance but, when presented with two directions of equal variance, the neuron tends to pick the one with larger negative Kurtosis. In particular, this fact allows the neuron to linearly separate bimodal inputs. Robustness to large input sizes (1000 inputs) is also studied, observing that the neuron is still able to find the principal component in a distribution under these conditions.

DY 13.17 Tue 9:30 P1

Fluctuations of Probe Particles Coupled to Molecular Motors — •Patrick Pietzonka, Eva Zimmermann, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

In recent years, many experiments have been carried out in which the motion of molecular motors is probed by the observation of attached colloidal particles. For the experimental determination of the torque exerted by the rotational motor F_1-ATPase onto such a particle, the application of a fluctuation theorem (FT) for the motion of the colloid has been proposed [1].

However, we show that this approach is generally valid only in the limit of fluctuations on short timescales. The statistics of fluctuations during larger time-intervals depends significantly on the intrinsic behavior of the motor and the linker, which is not observable in experiments. In particular, we investigate a simple model characterized by discrete motor jumps and harmonic coupling between the motor and the colloid [2]. Using the framework of the theory of large deviations, we calculate the distribution of fluctuations of the colloid in the long-time limit. This result implies a refined formulation of the FT-like relation observed in experiments. Moreover, we gain general insight into the properties of stochastic processes with hidden degrees of freedom.

[1] K. Hayashi *et al.*, Phys. Rev. Lett. **104**, 218103 (2010)
[2] E. Zimmermann and U. Seifert, New J. Phys. **14**, 103023 (2012)

DY 13.18 Tue 9:30 P1

Detention time of a model microswimmer at a plane surface: importance of hydrodynamic interactions — •Konstantin Schaar, Andreas Zöttl, and Holger Stark — TU Berlin, Institut für Theoretische Physik

We discuss the detention time of a microswimmer at a plane no-slip surface taking into account hydrodynamic interactions of the swimmer with the surface and rotational diffusion. To evaluate the detention time, we use the formalism of the mean first-passage time (MFPT) based on an appropriate Smoluchowski equation. The microswimmer operates in 'squirmer' mode and can easily be tuned between a 'pusher' and a 'puller'. The hydrodynamic interactions with the surface are described by lubrication theory.

We examine the MFPT and also the distribution of first passage times at the surface and achieve good agreement of our results with direct simulations of the squirmer motion close to the no-slip surface using the method of multi-particle collision dynamics. The detention time of the squirmer is clearly determined by hydrodynamic interactions with the surface. They rotate the squirmer away from the surface and therefore reduce the detention time considerably compared to pure rotational diffusion. We find that pushers have a larger detention time than pullers.

DY 13.19 Tue 9:30 P1

Thermodynamically consistent coarse graining of molecular motor models — •Eva Zimmermann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

In many single molecule experiments probe particles that are attached to molecular motors are used to infer properties of the motor protein from the analysis of the particle's trajectory and to manipulate the system by exerting external forces on the motor protein via the probe particle. Theoretical modelling used to describe such assays should comprise at least two coupled degrees of freedom. However, many simple theoretical models applied to molecular motor experiments contain only one degree of freedom representing the motor.

We use a simple illustrative model consisting of two coupled degrees of freedom for the molecular motor and the probe particle to introduce a coarse graining method that allows to eliminate the explicit dynamics of the probe particle in a dynamically and thermodynamically consistent way. We discuss under which conditions the coarse grained model reduces to the widely-used one-particle models.

DY 13.20 Tue 9:30 P1

Active Turing Systems — •Silke Bergeler, Florian Thüroff, and Erwin Frey — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München

Active Turing systems combine the ideas of active matter and reaction diffusion systems showing Turing patterns. We investigate such systems analytically and numerically starting within the framework of Boltzmann-like equations. Adapting previous analytical approaches for active systems we derive a set of hydrodynamic equations and perform a linear stability analysis of the isotropic uniform steady state. We find that the stability against homogeneous perturbations switches from unstable to stable by crossing a threshold noise from below. From direct simulations of the Boltzmann equation we observe that activity changes the form of the Turing patterns and broadens the parameter range for which patterns emerge. Analytical investigations on the stability of the isotropic homogeneous steady state are confirmed by numerical analysis.

DY 13.21 Tue 9:30 P1

Application of a random fitness landscape model to a long term evolution experiment — •Mares Barekzai[1], Su-Chan Park[2], and Joachim Krug[3] — [1]Department of Physics, University of Cologne,Germany — [2]Department of Physics, Catholic University of Korea, Bucheon, South Korea — [3]Department of Physics, University of Cologne,Germany

Since 1988, a long term microbial evolution experiment has attracted attention in the scientific community. In the experiment 12 populations of Escherichia coli are propagated in a daily refreshed minimal medium for more than 50000 generations. One of many results are the fitness trajectories of these asexually evolving populations, where fitness is measured as relative growth rate compared to the founding population. Is there a simple model to interpret the observed microbial evolution? We approached this question using the House of Cards Model introduced in 1978 by Kingman, which models the evolution of an asexual population on an uncorrelated random fitness landscape in the limit of infinite genome size. This limit implies that all mutations generate new fitness values drawn from a fixed probability distribution. The model produces fitness trajectories that are in qualitative agreement with the experimental data. Based on an analytical solution for the long term behavior of the model, we estimate the model parameters from the experimental data and provide a biological interpretation of our results.

DY 13.22 Tue 9:30 P1

Event chain simulations of polymer bundles — •Tobias Alexander Kampmann and Jan Kierfeld — TU Dortmund, Germany, NRW

We study simulation methods for large polymer systems forming locally dense structures such as polymer or filament bundles. In order to simulate such systems effectively using Monte-Carlo methods, we propose a novel event chain algorithm adapted from hard sphere systems [E. P. Bernard, W. Krauth, Phys. Rev. E, 80: 056704 (2009)]. The algorithm works rejection-free and reduces autocorrelation and equilibration times significantly.

We demonstrate the advantages of the algorithm by investigating the diffusive behaviour of bundle structures. Using the event chain algorithm a polymer bundle exhibits the correct scaling of diffusion constants with bundle size, which is not obtained using simple local displacement moves. We apply the algorithm to bundle networks formed by semiflexible filaments with short-range attractive interactions.

DY 13.23 Tue 9:30 P1

Estimation of sleep stages and sleep depth dynamics by neural clustering — •Stephan Volkland[1] and Jens Christian Claussen[2,1] — [1]INB, Universität zu Lübeck, Germany — [2]Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

The quantitative analysis of sleep from polysomnographic date (i.e., simulataneous recording of EEG, EMG and EOG) is practically limited by the final step of sleep scoring, i.e. extensive manual inspection of data according to the Rechtschaffen and Kales rules or the recent AASM counterpart, leading to a manually classified time series of sleep stages on a discrete scale of six values (wake, REM, S1, S2, S3, S4). Starting from the observation that the stages S2, S3, and S4 are merely defined by spectral properties, namely by activity in the delta and sigma band, here we present a neural clustering approach to assess sleep stages automatically by unsupervised neural clustering and a posteriori assignment of sleep stages. One particular goal is to provide a finer resolution in time as well as a finer interpolation in sleep depth than obtainable from manual scoring. We find that EOG and EMG data are still needed to improve classification of wake and REM states, and still an interpolation of states at the borders of wake, REM and S1 is difficult. In the range between the NonREM stages S1–S4 an interpolation with higher resolution is feasible, as expected.

DY 13.24 Tue 9:30 P1

Extended diffusion model of sleep depth dynamics — •Anna Barkentien[1] and Jens Christian Claussen[2,1] — [1]INB, Universität zu Lübeck, Germany — [2]Computational Systems Biology Lab, Research II, Jacobs University Bremen, Germany

The duration of wake bouts during sleep has puzzled complex systems scientists since a decade since [1], as these distributions eventually resemble a power-law. The theoretical understanding is incomplete, biologically plausible models still are not available. A pure Markov analysis [2] assuming random switching however ignores any deterministic components in the dynamics which are manifest in time correlations. The phenomenological model proposed in [1] describes sleep depth by a one-dimensional diffusion process with a reflecting border for sleep and a restoring force for wake. We extend this model in [3] to account for the REM state and modify the restoring force law to account for deviations to the power law that are observed in data from some (but not all) labs and obtain a better fit to data [3]. We conclude that a refined model as [3] is necessary to account for the different experimental results, but significantly larger cohorts of sleep studies would be needed to distinguish between the two-regime and the one-regime distributions. This concerns only the wake → sleep transition, the sleep → wake transition remains consistant with a random process homogeneous in time.
[1] C.C. Lo et al, EPL 57, 631, 2002. [2] J.W. Kim et al, PRL 102, 2009. [3] A. Barkentien and J.C. Claussen (in preparation).

DY 13.25 Tue 9:30 P1

Multidimensional epistasis and the transitory advantage of sex — •Johannes Neidhart, Stefan Nowak, Ivan G. Szendro, and Joachim Krug — THP, Universität zu Köln, Deutschland

The benefit of sex and recombination is a long standing problem. We numerically study evolutionary dynamics on high dimensional epistatic fitness landscapes, with focus on the temporal development of the evolutionary advantage of recombination. We show that the adaptive advantage of recombination on static landscapes is strictly transitory. These findings are explained by means of well established results for a setup with two loci. It is further shown that the transitory advantage can be prolonged indefinitely in fluctuating environments.

DY 13.26 Tue 9:30 P1

Adaptive walks in Kauffman's NK-Landscape — •Stefan Nowak and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Deutschland

We study evolutionary dynamics in a high-dimensional genotype space in the limit of rare mutations and strong selection. In this regime the population performs an uphill walk which terminates at local fitness optima. We analyze the length and attained fitness of such walks with our focus on the influence of different genetic interaction patterns.

DY 13.27 Tue 9:30 P1

Coexisting autocatalysts generate increasing complexity — •Emanuel Gregor Worst[1], Philipp Zimmer[2], Eva Wollrab[1], Karsten Kruse[2], and Albrecht Ott[1] — [1]Biologische Experimentalphysik, Universität des Saarlandes, Deutschland — [2]Theoretische Biologische Physik, Universität des Saarlandes, Deutschland

The evolution towards more complex structures from the earliest building blocks of life remains poorly understood. Here we present an experimental realization that exhibits evolutionary properties in one dimension and generates multiple coexisting species. Molecular chains of a certain length (identified as a species) are autocatalytically reproducing, and new species form randomly by spontaneous concatenation. We use DNA strands and DNA ligase, covalently linking single-stranded DNA, as an experimental model system. Reproduction occurs by template-directed ligation. Spontaneous and random generation of new species is a consequence of thermal fluctuations. We show that the system evolves towards more complex structures in a non-trivial way if the ratio between autocatalytic reproduction and spontaneous generation of new species exceeds a critical value. An outstanding characteristic of this system is the iterated production of more complex species while coexistence is maintained.

DY 13.28 Tue 9:30 P1

Identifying molecular expression dynamics in practice - how to distinguish between noise regulation and direct deterministic control using experimental data — •Martin Hoffmann[1] and Jörg Galle[2] — [1]Fraunhofer ITEM, Project Group Personalized Tumor Therapy, Biopark I, Josef-Engert-Strasse 9, 93053 Regensburg, Germany — [2]Interdisciplinary Centre for Bioinformatics, University of Leipzig, Haertelstr. 16-18, 04107 Leipzig, Germany

Biological noise plays an important role in generating phenotypic diversity and contributes to unspecific environmental adaptation. However, the classical pathway view of cell biology focusing on deterministic stimulus-response relationships may well accommodate the majority of biological phenomena. It is thus necessary to develop combined theoretical and experimental approaches that can dissect the relative contribution of noise regulation and direct deterministic control. Accordingly, we define molecular level conditions for noise-driven and deterministic dynamics and compare corresponding modeling results to published experimental data. We show that both models can fit the FACS data for the toggle switch system equally well while simulated dynamic mRNA labeling results in distinct observations for both models. Using synthetic time course data we demonstrate that complete system identification can be achieved based on single cell tracking. As demonstrated, noise regulation can be an effective second layer of cell regulation that may be associated with active short term search processes.

DY 13.29 Tue 9:30 P1

Propagation and propagation failure of waves on excitable tree networks — Nikos Kouvaris[1], •Thomas Isele[2], Alexander Mikhailov[3], and Eckehard Schöll[2] — [1]Department of Physics, University of Barcelona, Marti i Franques 1, 08028, Barcelona, Spain — [2]Institut für theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [3]Department of Physical Chemistry, Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany

We study the properties of pulse solutions on excitable tree networks by means of numerical (simulation and continuation) as well as analytical methods. We focus on the dependence of the propagation velocity and the change of stability properties with respect to the branching

ratio (i.e. degree) of the nodes. But we also consider different coupling strengths and the continuous (thermodynamic) limit of our model.

DY 13.30 Tue 9:30 P1

Dynamics of neural networks with transient synaptic plasticity rules — •Bulcsú Sándor and Claudius Gros — Institut für Theoretische Physik, Goethe Universität, Frankfurt am Main, Deutschland

Working memory makes it possible to hold information temporarily for processing purposes; as such it has an important role in the execution of cognitive tasks. Its operation may possibly be mediated via short-term or transient synaptic plasticity effects. Thus the standard Tsodyks-Markram model for transient synaptic dynamics, built upon short-term synaptic plasticity effects, is a promising candidate to investigate the underlying dynamical behavior of these systems.

In our work we propose a simplified continuous time model for presynaptic plasticity rules, called full depletion model, which may allow a stricter control of the dynamics. The model is implemented for clique encoding recurrent networks with a Mexican-hat connection profile of synaptic weights. These systems show a wide variety of dynamical states as a function of the control parameters. We study the different types of behaviour emerging from transient synaptic plasticity rules from a dynamical system's point of view.

DY 13.31 Tue 9:30 P1

Optimization of complex network for minimizing traffic congestion: case study for a popular internet based service in Serbia — •Igor Stanković[1], Vladica Tinotor[2], and Jovan Radunović[3] — [1]Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [2]Republic Agency for Electronic Communications, Višnjićeva 8, 11000 Belgrade, Serbia — [3]School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia

We present a case study of network parameter optimization for a popular internet based service in Serbia. The physical layer of the network consists of two existing nation-wide optical networks, i.e., a commercial telecommunication network and a network of public power grid operator. The second network is build for synchronization and control of the power grid and is not currently used commercially. Information traffic is directed by standard Open Shortest Path First routing protocol and in our case initial link weights are assigned according to the link costs [1]. We apply optimization algorithm aimed at avoiding, if possible, link overload by a judicious link weight tuning. The output characteristics which enter into quality of service function are link utilization and total cost of the service. The input parameters of the optimization algorithm are network topology, relevant protocol, link costs and capacities.

[1] J. Smiljanic, I. Stankovic, "Efficient Routing on Small Complex Networks Without Buffers", Physica A **392**, (2013) 2294.

DY 13.32 Tue 9:30 P1

Motifs in Triadic Random Graphs Based on Steiner Triple Systems — •Marco Winkler and Jörg Reichardt — Institute for Theoretical Physics, University of Würzburg, Germany

Conventionally, pairwise relationships between nodes are considered to be the fundamental building blocks of complex networks. However, over the last decade so-called motifs have attracted much attention. It has been hypothesized that these motifs, rather than links, serve as the building blocks of network structures. Although the relation between a network's topology and its function, its robustness against perturbations, or its efficiency in spreading information, is the central theme of network science, there is still a lack of sound generative models needed for testing the functional role of subgraph motifs. Our work aims to overcome this limitation. We employ the framework of exponential random graph models (ERGMs) to define models based on triadic substructures. The fact that only a small portion of triads can actually be set independently poses a challenge for the formulation of such models. To overcome this obstacle, we use Steiner triple systems (STSs). These are partitions of sets of nodes into pair-disjoint triads, which thus can be specified independently. Combining the concepts of ERGMs and STSs, we suggest generative models capable of generating ensembles of networks with nontrivial triadic Z-score profiles. Further, we discover inevitable correlations between the abundance of triad patterns, which occur solely for statistical reasons and need to be taken into account when discussing the functional implications of motif statistics.

DY 13.33 Tue 9:30 P1

Architecture of biologically inspired adaptive transport networks — •Johannes Gräwer[1], Carl Modes[2], Marcelo O. Magnasco[2], and Eleni Katifori[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Laboratory of Mathematical Physics, The Rockefeller University, New York, NY, USA

We study self-organized adaptation mechanisms of biologically inspired transport networks (e.g. plasmodial veins of slime moulds). Therefore, evolving network architectures are simulated using a generic dynamical system and weighted graphs. The graphs' edges represent tubes with Hagen-Poiseuille flow, connected through junctions, represented by their nodes. A local update rule, that changes the conductivity of the tubes (edge weights) according to the flow through them, is used as a self-organizing adaptation principle. We model these interrelated transportation and adaptation processes on paradigmatic complex network topologies (e.g. Watts-Strogatz, Barabási-Albert, Erdös-Rényi) with random initial edge weights. We examine the adaptation dynamics and find, that it exhibits discrete, cascade reorganization events until the network reaches a hierarchically organized state.

DY 13.34 Tue 9:30 P1

Quantum walks on 1D and 2D quasi-crystals — •Chi-Hung Weng and Oliver Mülken — Institute of Physics, University of Freiburg, Germany

We study the dynamics of quantum walks on a quasi-crystals modelled by the tight-binding Aubry-André-Harper (AAH) equation. We numerically solved both the diagonal/off -diagonal AAH in both 1D and 2D cases. It is known that the 2D diagonal AAH can also be regarded as a model for the Integer Quantum Hall Effect (IQHE), a phenomena when a 2D electron gas is subjected to strong magnetic fields at a low temperature. As a consequence we also observe the edge states which are responsible for carrying the current. Those states can be changed from localized to de-localized, as a topological phase within the aperiodic modulated on-site potential varies. In order to identify how localized the states are, as well as how fast the transport is, the Inverse Participation Ratio (IPR) and Mean Squared Displacement (MSD) are calculated, respectively. Moreover, we also study the impact of disorder and non-Hermitian settings (i.e. system with absorbers or Parity-Time (PT) symmetric modulated aperiodicity) on the dynamics.

DY 13.35 Tue 9:30 P1

Transport efficiency in complex networks — •Marco Tabarelli and Oliver Mülken — Albert-Ludwigs-Universität, Freiburg, Germany

We examine complex networks of two-level quantum systems regarding their efficiency to transport exitons through the network. Our model uses the so-called Quantum Stochastic Walk (QSW), a version of a quantum master equation in Lindblad form (LME) which allows to parametrize the classical-quantummechanical crossover. To describe a circular probability current an external node is coupled to two "ends" of the network acting as a source to an entrance node and a trap to an exit node. These links are directed and their effect is realized with additional Lindblad operators in the dissipative term of the LME. Comparing stationary solutions of node populations sheds light on the probability current through the network. In addition to the geometry of the network, parameters varied include the internal coupling constant, source- and trap strength and the ratio of coherent and decoherent transitions. Networks studied include modified linear chains and networks with self-similarity properties.

DY 13.36 Tue 9:30 P1

Feedback control of vorticity in a Newtonian fluid — •Maria Zeitz and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin

Our goal is to explore feedback control strategies to stabilize novel dynamic flow patterns in microfluidic model systems. As an example, we investigate a Couette flow geometry without the inner cylinder filled with a Newtonian fluid. Its vorticity satisfies a diffusion equation. To stabilize a mean vortex strength in the flow field, we use feedback control with hysteresis. We either set the angular velocity of the outer cylinder or apply a torque at the boundary and switch velocity or torque value in a hysteretic fashion depending on the actual mean vortex strength. Since the boundary condition changes with time, the system does not reach a stationary state. In this setup, we explore

the possibility of time-periodic solutions and spatial flow patters. In a second step, we will also implement time-delayed feedback in our system.

DY 13.37 Tue 9:30 P1

Fractal distributions in a cyclic information-engine with optimal feedback — •Michael Bauer, Andre C. Barato, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

It is known that information obtained by measurements can be converted into work, the paradigmatic example being Szilard's engine. For a two level system coupled to a heat bath and a work reservoir we obtain the optimal protocol corresponding to the maximal work extraction. Moreover, we consider a controller performing cyclic measurements and changing the protocol accordingly. Analyzing this optimal cyclic machine we find a recursion relation for the initial occupation probability of the level with higher energy, which depends on the measurement error. Through the numerical analysis of this relation we obtain a fractal histogram, which is a strange attractor (common in chaos theory). This fractal structure can be explained with a simplified model leading to the Cantor set.

DY 13.38 Tue 9:30 P1

Feedback control of non-equilibrium dynamics of a multi-layer system of confined colloidal particles in planar shear flow — •Sascha Gerloff, Tarlan A. Vezirov, and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

We perform computer simulations of charged colloidal particles in planar shear flow combined with feedback control. The particles interact via a combined Yukawa- and softsphere-potential. The system is known to form shear-induced multi-layer configurations in confinement and to show different intra-layer structures which depend on the applied shear rate [1]. The parameters are set to suit experimental data for ludox silica particles, which where previously studied [2, 3].
We employ overdamped Brownian dynamics simulations to investigate the structure and the rheological behavior of the considered system. We then supplement our equations of motion by an additional dynamical equation, which corresponds to a feedback control mechanism for the shear rate via the shear stress. This enables the system to select between steady states dependent on the control parameters. Furthermore we present an approximation which estimates the transtion between steady states in the control parameter space analytically.
[1] T. A. Vezirov and S. H. L. Klapp, Phys. Rev. **E 88**, 5 (2013).
[2] S. Grandner and S. H. L. Klapp, J. Chem. Phys. **129**, 244703 (2008).
[3] S. H. L. Klapp, Y. Zeng, D. Qu and R. v. Klitzing, Phys. Rev. Lett. **100**, 118303 (2008).

DY 14: Networks, From Topology to Dynamics I (joint session SOE/DY/ BP)

Time: Tuesday 15:00–16:00 Location: GÖR 226

DY 14.1 Tue 15:00 GÖR 226

The Hidden Geometry of Complex, Network-Driven Contagion Phenomena — •Dirk Brockmann[1,2] and Dirk Helbing[3] — [1]Humboldt University, Berlin — [2]Robert Koch Institute, Berlin — [3]ETH Zurich

The global spread of epidemics, rumors, opinions, and innovations are complex, network-driven dynamic processes. The combined multiscale nature and intrinsic heterogeneity of the underlying networks make it difficult to develop an intuitive understanding of these processes, to distinguish relevant from peripheral factors, to predict their time course, and to locate their origin. We show that complex spatiotemporal patterns can be reduced to surprisingly simple, homogeneous wave propagation patterns, if conventional geographic distance is replaced by a probabilistically motivated effective distance[1]. In the context of global, air-traffic-mediated epidemics, we show that effective distance reliably predicts disease arrival times. Even if epidemiological parameters are unknown, the method can still deliver relative arrival times. The approach can also identify the spatial origin of spreading processes. We validate the approach by application to data on the worldwide 2009 H1N1 influenza pandemic, the 2003 SARS epidemics and the 2011 outbreak of EHEC/HUS in Germany.
D. Brockmann, D. Helbing, Science (2013)

DY 14.2 Tue 15:15 GÖR 226

Spread of Infectious Diseases with Finite Infectious Period on Temporal Networks — •Andreas Koher, Lucian Willareth, Hartmut Lentz, and Igor M. Sokolov — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Traversal in temporal networks is only possible, if paths are formed by a causal sequence of edges. Recently, a matrix formalism has been introduced in order to compute the causal path structure of temporal networks [1]. This formalism describes the spread of infectious diseases that can traverse the network even after arbitrary waiting times, i.e. a SI-model (susceptible-infected-model). Many infectious diseases however possess a finite infectious period, i.e. the time period after which the infection dies out, if it is not passed on. This can be implemented as an SIS or SIR (susceptible-infected-recovered) model, respectively. In this work, we introduce a novel matrix formalism that allows for an explicit consideration of finite infectious periods, which gives a more realistic model of outbreak scenarios. As a central result, we compute the critical infectious period necessary in order to allow for percolation on a given temporal network. The introduced methods can be implemented efficiently and we demonstrate their capability on different datasets.
[1] Lentz et al., Unfolding Accessibility Provides a Macroscopic Approach to Temporal Networks, Phys. Rev. Lett. (2013)

DY 14.3 Tue 15:30 GÖR 226

Dynamics of Manufacturing Supply Networks — •Thilo Gross — University of Bristol

High-value manufacturing builds on increasingly complex supply networks. In contrast to classical supply chains these networks have a high connectivity and can contain loops and hubs. Failure of the supply network can cause business disruptions associated with high financial losses. Presently, already more than 30% of such losses are caused by cascading effects that propagate through the system. In the face of this threat mathematical tools are needed to assess the robustness and resilience of supply networks and identify vulnerabilities. In this talk I present modelling approaches and results on the stability of dynamical manufacturing supply networks. In particular, I identify potential bifurcations of the network and propose a method to identify the most critical suppliers in large networks.

DY 14.4 Tue 15:45 GÖR 226

Automatic discovery of plausible network models — Telmo Menezes[1,2] and •Camille Roth[1] — [1]Centre Marc Bloch Berlin, CNRS — [2]Centre d'Analyse et de Mathématique Sociales, CNRS/EHESS

A methodology is proposed to discover plausible network generators for complex networks. Generators are defined as computer programs that define local morphogenetic behaviors. We employ a machine learning technique inspired by biological Darwinism to look for generators that produce synthetic networks which match a number of metrics on target real networks. We use a number of metrics that capture both global and fine-grained structural characteristics of networks. Remarkably, when applied on networks stemming from prototypical models of the Erdös-Rényi or Barabási-Albert sort, our approach generally discovers the exact original generator. Empirical validation of our methodology is then presented in the form of a number of plausible generators for a series of five real networks, including a simple brain and a social network.

DY 15: Nonlinear Dynamics, Synchronization and Chaos - Part I

Time: Wednesday 9:30–11:45 Location: HÜL 186

DY 15.1 Wed 9:30 HÜL 186

Coherent-structure theory for non-local generalised Kuramoto-Sivashinsky eqautions — Te-Sheng Lin[1], •Dmitri Tseluiko[1], Marc Pradas[2], Serafim Kalliadasis[2], and Demetrios Papageorgiou[2,3] — [1]Department of Mathematical Sciences, Loughborough University, UK — [2]Department of Chemical Engineering, Imperial College London, UK — [3]Department of Mathematics, Imperial College London, UK

We analyse coherent structures in non-local active-dissipative equations, using as a prototype a generalised Kuramoto-Sivashinsky (gKS) equation with a non-local term that is assumed to be a pseudo-differential operator with a spatially independent symbol. Such equations arise in various physical contexts, e.g. in the modelling of a liquid film flow in the presence of various external effects. As for the gKS equation, we show that dispersion regularises the chaotic behaviour and the solutions evolve into arrays of interacting pulses that can form bound states. Since the Shilnikov-type approach is not applicable for analysing bound states in non-local equations, we develop a weak-interaction theory. The non-locality changes the decay of the tails of the pulses from exponential to algebraic. This has strong influence on pulse interaction and bound-state formation, e.g., unlike for local equations, for a correct description of the interaction of pulses it is not sufficient to take into account only neighbouring pulses, in addition interactions become stronger and bound-state formation is speeded up, moreover the number of possible bound states is always finite. Theoretical predictions are corroborated by numerical experiments.

DY 15.2 Wed 9:45 HÜL 186

Multiplicity of Singular Synchronous States in the Kuramoto Model of Coupled Oscillators — •Maxim Komarov and Arkady Pikovsky — Department of Physics and Astronomy, Universität Potsdam, Karl-Liebknecht-Str 24/25, Bld. 28 D-14476 Potsdam, Germany

We study the Kuramoto model of globally coupled oscillators with a bi-harmonic coupling function. We develop an analytic self-consistency approach to find stationary synchronous states in the thermodynamic limit, and demonstrate that there is a huge multiplicity of such states, which differ microscopically in the distributions of locked phases. These synchronous regimes exist already prior to linear instability transition of the fully asynchronous state. In the presence of white Gaussian noise the multiplicity is lifted, but the dependence of the order parameters on coupling constants remains nontrivial.

DY 15.3 Wed 10:00 HÜL 186

Pattern formation in the synchronization dynamics of arrays of optomechanical oscillators — •Roland Lauter, Christian Brendel, Max Ludwig, Steven Habraken, and Florian Marquardt — Institut für Theoretische Physik II, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstraße 7 91058 Erlangen

We consider two-dimensional arrays of coupled optomechanical cells, each of which consists of a laser-driven optical cavity interacting with a mechanical (vibrational) mode. The mechanical modes can be driven in self-sustained oscillations. We study the collective classical nonlinear dynamics of the phases of these oscillations, which is described by the well-studied Kuramoto model and optomechanical extensions thereof. The model parameters can be tuned by the laser drives. We focus on pattern formation and find that, depending on the parameters, the phases may or may not synchronize in a stationary configuration of vortex-antivortex pairs. We identify a relevant length scale and find hysteresis associated to the synchronization transition. For some model parameters, this length scale becomes comparable to the lattice spacing, in which case the phase configurations develop structure on smaller and smaller scales and eventually settle into random patterns. Besides, we address the stability and time evolution of binary patterns in which all oscillators are initialized to phases of 0 or pi.

DY 15.4 Wed 10:15 HÜL 186

Simple mechanism for controlling pattern formation in coupled genetic circuits — •Darka Labavić, Prabesh Joshi, and Hildegard Meyer-Ortmanns — School of Engineering and Science, Jacobs University Bremen

We study a system of coupled genetic circuits - bistable frustrated units. Individual units show excitable or oscillatory behaviour depending on the choice of parameters [1]. The same regimes are present also for coupled units, with the same bifurcation parameter. Tuning this parameter we can generate pattern formation for a finite duration of time. Depending on the tuning speed, network topology, and coupling strength, we observe a rich dynamics with different time scales, self-organized pacemakers, spiral patterns, and planar waves. To demonstrate the complexity of the dynamics, we do a detail bifurcation analysis on two coupled units, and indicate how it extrapolates to a larger network.

[1] P. Kaluza and H. Meyer-Ortmanns, Chaos **20**, 043111(2010)

15 min break

DY 15.5 Wed 10:45 HÜL 186

Stuart-Landau oscillators with a conservation law: chimera states and clustering — •Lennart Schmidt[1,2], Katharina Krischer[1], and Vladimir García-Morales[1] — [1]Physik-Department, Nonequilibrium Chemical Physics, Technische Universität München, Garching, Germany — [2]Institute for Advanced Study - Technische Universität München, Garching, Germany

We describe a population of Stuart-Landau oscillators with a nonlinear global coupling. This coupling leads to conserved harmonic oscillations of the mean field. In simulations we observe various kinds of dynamics, including two types of chimera states. Furthermore, tuning the amplitude of the mean-field oscillations gives rise to a transition from the synchronized state to clusters via a Hopf bifurcation. At the Hopf bifurcation two groups emerge out of the whole population, oscillating in anti-phase as to fulfill the conservation law. Since in general the frequency of the new limit cycle is incommensurate to the frequency of the mean-field oscillations, one observes quasiperiodic dynamics.

DY 15.6 Wed 11:00 HÜL 186

Robustness of chimera states in neural system — •Iryna Omelchenko[1,2] and Philipp Hövel[1,2] — [1]Institut für Theoretische Physik, Technische Universität Berlin — [2]Bernstein Center for Computational Neuroscience, Humboldt-Universität zu Berlin

Chimera states are peculiar patterns characterized by coexistence of spatial regions with regular synchronized and irregular incoherent motion in systems of nonlocally coupled elements. We investigate the cooperative dynamics of nonlocally coupled neural populations modeled by FitzHugh-Nagumo systems, where each individual system displays oscillatory local dynamics. In this system, next to the classical chimera state, which exhibits one coherent phase-locked and one incoherent region, we find a new class of dynamics that possesses multiple domains of incoherence [1].

To address the question of robustness of chimera states, inhomogeneity of the local units is introduced in the system via a distribution of threshold parameters of individual FitzHugh-Nagumo oscillators. In dependence on the inhomogeneous system's parameter distribution, we analyze existence of chimera and multi-chimera states in the system.

[1] I. Omelchenko, O.E. Omel'chenko, P. Hövel, and E. Schöll. Phys. Rev. Letters 110, 224101 (2013).

DY 15.7 Wed 11:15 HÜL 186

Clustered Chimera States in Systems of Type-I Excitability — •Andrea Vüllings[1], Johanne Hizanidis[2], Iryna Omelchenko[1,3], and Philipp Hövel[1,3] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]National Center of Scientific Research "Demokritos", Agia Paraskevi, 15310 Athens, Greece — [3]Bernstein Center for Computational Neuroscience, HU Berlin, Philippstr. 13, 10115 Berlin, Germany

Chimera is a fascinating phenomenon of coexisting synchronized and desynchronized behaviour discovered in networks of nonlocally coupled identical phase oscillators more than ten years ago. Since then, chimeras were found in numerous theoretical and experimental studies and more recently in models of neuron dynamics as well [1,2]. In this work, we consider a generic model for a saddle-node bifurcation on a limit cycle representative for neuron excitability type I. We obtain chimera states with multiple coherent regions (clustered chimeras) depending on the distance from the excitability threshold as well as the range of nonlocal coupling. A detailed stability diagram for these

chimera states as well as other interesting coexisting patterns like travelling waves will be presented. Finally, in order to gain more insight into the observed dynamics we will employ a modified Kuramoto phase oscillator model as a good approximation to our system above the bifurcation point.

[1] I. Omelchenko *et al.*, *Phys. Rev. Lett.* **110**, 224101 (2013).
[2] J. Hizanidis *et al.*, *Int. J. Bif. Chaos* (2013).

DY 15.8 Wed 11:30 HÜL 186

Robustness of Chimera States in Nonlocally Coupled Networks of Nonidentical Logistic Maps — •Anne-Kathleen Malchow[1], Philipp Hövel[1,2], and Iryna Omelchenko[1,2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Bernstein Center for Computational Neuroscience, Humboldt-Universität zu Berlin, Philippstraße 13, 10115 Berlin, Germany

We investigate the spatio-temporal dynamics of a ring-network of nonlocally coupled discrete maps, where each element is coupled to a certain number of nearest neighbors. The local dynamics are described by logistic maps with nonlinearity parameters drawn from some fixed distribution within the chaotic regime.

Besides synchronous and spatially chaotic states, we focus particularly on the existence of spatially coherent solutions as well as on the presence of multistable chimera-like states at the transition from coherence to incoherence. Chimera-like states are characterized by a hybrid spatial structure, as they are partially coherent and partially incoherent.

Varying the range and strength of the coupling and especially the variance of the distribution of the nonlinearity parameter values, which denotes the extent of inhomogeneity in the system, we analyze the stability of the different states and compare their stability regions with the case of identical elements.

DY 16: Statistical Physics in Biological Systems (joint session DY/ BP)

Time: Wednesday 9:30–12:00 Location: ZEU 160

DY 16.1 Wed 9:30 ZEU 160

Statistics of local multiple sequence alignments — •Pascal Fieth and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

To assess the significance of alignment scores obtained by comparing DNA or amino acid sequences using sequence alignment, knowledge of the score distribution in the biologically relevant high-scoring region is necessary. The score distribution can analytically be shown to follow a Gumbel extreme value distribution for gapless local alignments. For gapped alignments, however, the distribution can only be obtained numerically. To cover the rare-event region of the distribution, studies of the score distribution of pairwise local alignments were done utilising parallel tempering[1]. They showed that, unlike predicted by previous simple sampling approaches, a Gaussian correction to the Gumbel distribution is necessary in case of finite sequence lengths. Here, this study is expanded to sum-of-pair scores of multiple sequence alignments, i.e. the alignments of more than two sequences, with gaps. Results will be shown for the score distributions of local multiple alignments and compared to previous results for global multiple alignments, where regions with probabilities smaller than 10^{-70} could be obtained.

[1] S. Wolfsheimer, B. Burghardt, A.K. Hartmann, *Local sequence alignment statistics: deviations from Gumbel statistics in the rare-event tail*, Algorithms for Molecular Biology (2007)

DY 16.2 Wed 9:45 ZEU 160

Optimising the spatial structure of BLN protein models by means of "partial distortion"-quench cycles — •Florian Günther[1,2,3], Arnulf Möbius[2], and Michael Schreiber[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Institute of Physics, Technical University Chemnitz, Germany

The prediction of the spatial structure of a protein based on its amino acid sequence is a challenging problem. Corresponding theoretical studies of the protein folding require highly efficient structure optimisation tools. Here we investigate whether and to what extent the thermal cycling (TC) algorithm [1] is appropriate for determining low energy structures of the BLN protein model by J.D. Honeycutt and D. Thirumalai [2]. In our simulations for 46-, 58-, and 69-bead sequences, the TC algorithm reliably finds the global minimum within reasonable computing time. In comparison to the multi-start local search and simulated annealing approaches, TC turns out to be far more efficient.

In the present work, the BLN model with rigid bonds is studied in detail for the first time. Comparing these results to data for the extended model by Berry *et al.* [3], where stiff springs are substituted for the rigid bonds, we observe several level crossings when varying the spring constant, even for quite hard springs.

[1] A. Möbius *et al.*, Phys. Rev. Lett. **79** (1997) 4297.
[2] J.D. Honeycutt and D. Thirumalai, Biopolymers **32** (1992) 695.
[3] R.S. Berry *et al.*, Proc. Natl. Acad. Sci. USA **94** (1997) 9520.

DY 16.3 Wed 10:00 ZEU 160

Stochastic Processes with Delays and Their Application to Gene Regulation and Epidemics — •Tobias Brett and Tobias Galla — The University of Manchester, Manchester, United Kingdom

Many of the systems modeled in biology have memory: not all of the effects of interactions can be well approximated as occurring instantaneously. Examples are transcriptional and translational delays in gene regulation, or recovery periods in the context of infectious diseases. We focus on chemical reaction models with delays. For such processes it is not straightforward to formulate Master equations, and it is not clear how to derive systematic Gaussian approximations. We demonstrate that progress can be made using a path-focused view, based on generating functionals. These do not describe the time-evolution of one-time probability distributions, instead they capture the probabilities of entire paths. We derive analytical expressions for Gaussian approximations for a wide class of delay systems, and apply these to two biological problems in which delay is relevant. One is the susceptible-infective-recovered model in epidemiology and the other a model of delayed autoinhibition in gene regulation. This allows us to characterise the phenomena arising from the combination of intrinsic noise and delayed dynamics.

Reference: T. Brett, T. Galla, Phys. Rev. Lett. **110**, 250601 (2013)

DY 16.4 Wed 10:15 ZEU 160

Environmental effects on DNA denaturation — •Christian von Ferber[1] and Yurij Holovatch[2] — [1]AMRC, Coventry University, Coventry, UK — [2]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, Ukraine

We re-consider the Poland and Scheraga model for the DNA denaturation transition where the double DNA strands locally and then globally detach as the transition temperature is attained. Applying a polymer field theory approach we discuss in particular variants of this transition that may occur due to the properties of the environment. We show that different environments may shift the transition further or less towards a first order transition. Effects we discuss are: the presence of (1) uncorrelated and (2) power-law long-range correlated disorder where the latter influences the transition as function of the power law exponent,(3) quality of the solution which may affect the self- and mutual interaction of both single and double strands, and (4) combinations of these effects. We find that the effects studied significantly influence the transition.

15 min break

DY 16.5 Wed 10:45 ZEU 160

Pattern formation in individual-based systems with time-varying parameters — •Peter Ashcroft and Tobias Galla — The University of Manchester, Manchester, UK

We study the patterns generated in finite-time sweeps across symmetry-breaking bifurcations in individual-based models of evolutionary dynamics and cell differentiation. Similar to the well-known Kibble-Zurek scenario of defect formation, large-scale patterns are generated when model parameters are varied slowly, whereas fast sweeps produce a large number of small domains. The symmetry breaking is triggered by intrinsic noise, originating from the discrete dynamics at the microlevel. Based on a linear-noise approximation, we calculate the

characteristic length scale of these patterns. We demonstrate the applicability of this approach in a model of evolutionary game theory with a time-dependent fitness structure, and in a model of cell differentiation, which we relate to Waddington's epigenetic landscape. Our theoretical estimates are confirmed in simulations. In further numerical work, we observe a similar phenomenon when the symmetry-breaking bifurcation is triggered by population growth.

Reference: P. Ashcroft and T. Galla, Phys. Rev. E 88, 062104 (2013)

DY 16.6 Wed 11:00 ZEU 160

A time-continuous model for E. coli's motion using shot noise — •Oliver Pohl[1], Marius Hintsche[2], Carsten Beta[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, 14476 Potsdam, Germany

The bacterium Escherichia coli moves with alternating runs and tumbles that occur with a mean tumble rate. In the presence of gradients of a chemoattractant, E. coli performs chemotaxis [1]. It adjusts the tumble rate in response to the time-integrated concentration in order to increase the uptake of the chemical.

We set up a time-continuous model that describes runs and tumbles as a stochastic process of the bacterium's swimming direction and speed. The swimming direction updates according to rotational Brownian motion and additional shot noise, which initiates tumbling events. The speed is not constant as in previous models but is determined by the random shots as well. By analyzing experimental data on swimming trajectories, we adjust the parameters of our model. First, we determine the shot noise from higher moments of the experimental trajectories. Second, we present a novel approach to determine the chemotactic response function, which E.Coli uses to integrate the chemical concentration in time. Finally, we want to use our model to explore the behavior of E. Coli in different chemical concentration profiles.

[1] H.C. Berg, "E.Coli in motion", Springer, New York, (2003)

DY 16.7 Wed 11:15 ZEU 160

Self-propelled particles with alignment and anti-alignment — •Robert Grossmann[1], Pawel Romanczuk[1], Markus Bär[1], and Lutz Schimansky-Geier[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Department of Physics, Humboldt-Universität zu Berlin, Germany

It was recently suggested that the observations of vortex structures in the local polarization of dense bacterial suspensions can be explained by a negative viscosity in the hydrodynamic equation for the polar order parameter [1]. Here, we propose a simple model of self-propelled particles interacting via a short-ranged alignment and a long-ranged anti-alignment, which may exhibit negative viscosity. This simple model allows us to systematically derive a coarse-grained description via a one-particle Fokker-Planck equation [2], and to analyze the relation of hydrodynamic transport coefficients on the microscopic parameters of the model. We explore the impact of different approximations required in the derivation of the coarse-grained theory on the validity of the linearized equations. Furthermore, we verify our results by comparing numerical simulations of the microscopic model with predictions of the coarse-grained theory.

[1] Dunkel, J. et al., New J. Phys., 15, 045016 (2013)
[2] Grossmann, R. et. al, New J. Phys., 15, 085014 (2013)

DY 16.8 Wed 11:30 ZEU 160

Constructing a Stochastic Model of Bumblebee Flights from Experimental Data — Friedrich Lenz[1], Aleksei V. Chechkin[2], and •Rainer Klages[1] — [1]Queen Mary U. of London, School of Math. Sci., UK — [2]Inst. f. Theor. Physics, NSC KIPT, Kharkov, Ukraine

The movement of organisms is subject to a multitude of influences of widely varying character: from the bio-mechanics of the individual, over the interaction with the complex environment many animals live in, to evolutionary pressure and energy constraints. As the number of factors is large, it is very hard to build comprehensive movement models. Even when movement patterns in simple environments are analysed, the organisms can display very complex behaviours. While for largely undirected motion or long observation times the dynamics can sometimes be described by isotropic random walks, usually the directional persistence due to a preference to move forward has to be accounted for, e.g., by a correlated random walk. We generalise these descriptions to a model in terms of stochastic differential equations of Langevin type, which we use to analyse experimental search flight data of foraging bumblebees [1]. Using parameter estimates we discuss the differences and similarities to correlated random walks. From simulations we generate artificial bumblebee trajectories which we use as a validation by comparing the generated ones to the experimental data [2]

[1] T.C.Ings, L.Chittka, Curr. Biol. **18**, 1520 (2008)
[2] F.Lenz, A.V.Chechkin, R.Klages, PLoS ONE **8**, e59036 (2013)

DY 16.9 Wed 11:45 ZEU 160

Swarming of self-propelled agents with selective attraction-repulsion interaction - From microscopic dynamics to coarse-grained theories — •Pawel Romanczuk[1], Robert Grossmann[1], and Lutz Schimansky-Geier[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin — [2]Department of Physics, Humboldt Universität zu Berlin

We propose a model of stochastic self-propelled agents interacting via selective attraction-repulsion interaction, where individuals respond differently to their neighbours depending on their relative state of motion (approach versus movement away) [1]. This kind of social response is directly motivated by visual sensory information available to individuals (e.g. looming stimuli). We show that the model exhibits various modes and collective behaviour and derive a coarse-grained description via a non-linear Fokker-Planck equation, which allows us to formulate hydrodynamic equations for the density and velocity fields of the Toner-Tu type [2]. Finally, we compare the predictions on the linear stability from our coarse-grained theory with the results of individual-based simulations of the microscopic model, and discuss the limitations of the hydrodynamic theory and its region of validity.

[1] Romanczuk P. and Schimansky-Geier L., Interface Focus 2, 746-756 (2012)
[2] Grossmann R., Schimansky-Geier L., Romanczuk P., New J Phys 15, 085014, (2013)

DY 17: Modeling and Data Analysis

Time: Wednesday 9:30–11:45 Location: ZEU 146

DY 17.1 Wed 9:30 ZEU 146

Analytical solutions for a model of tow-phase-flow in porous media — •Christoph Wolber and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, 70569 Stuttgart

Modeling immiscible two-phase flow in porous media on a macroscopic scale has proven difficult due to hysteresis and residual saturation. The traditional Buckley-Leverett- theory has to resolve these difficulties by explicitly introducing hysteresis into core concepts like capillary pressure and relative permeability. A new approach distinguishes between percolating and non percolating components of the fluid phases (2006b Phys. Rev. E 73 016307). The hysteresis is reproduced and can be linked to the entrapped fluids that are the physical cause of it. Analytical solutions for a hyperbolic limit have been studied with the method of characteristics. They show shocks and rarefaction waves as expected of hyperbolic partial differential equations. In addition to reproducing the results of the traditional theory where they are valid, the new theory can model processes where imbibition and drainage take place at the same time at different sites as well as flow-reversal problems.

DY 17.2 Wed 9:45 ZEU 146

Generation of drainage or imbibition waves from nonconstant initial saturations of trapped disconnected fluid parts during two-phase immiscible displacement — •Rouven Steinle and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Deutschland

For two-phase immiscible displacement in a homogeneous porous medium with spatially constant initial saturation the traditional Darcy theory predicts no changes of the saturations during drainage or imbibition when the boundary saturations are kept constant. The physical content of a recent generalization of the traditional Darcy theory is tested by studying a similar initial and boundary value problem. The generalized theory distinguishes between percolating and nonpercolating (trapped, disconnected) fluid phases [1]. The initial value problem now requires to specify initial profiles separately for the percolating and nonpercolating phases. When the initial nonpercolating profiles are position dependent drainage or imbibition waves may be generated depending on the initial profiles [2]. These results allow to test the generalized theory by comparing its predictions to experiment.

[1] R. Hilfer, *Macroscopic capillarity without a constitutive capillary pressure function*, Physica A, vol. 371, pp. 209, (2006)

[2] A. Monge Sánchez, *Numerical Solutions of Macroscopic Equations for Multiphase Flows in Porous Media*, Master Thesis, (2013)

DY 17.3 Wed 10:00 ZEU 146

Iterative Modellierung elektronischer Verteilungsfunktionen – Auf dem Weg zur Lumineszenz — •Juri Romazanov, Mourad el Kharrazi, Orkhan Osmani und Marika Schleberger — Fakultät für Physik, Universität Duisburg-Essen, Duisburg

Bis heute gibt es keine einheitliche Beschreibung der Dynamik des Elektronengases im Festkörper nach einer Anregung durch schwere, schnelle Ionen ($E > 1$ MeV/u). Ein häufig verwendeter Ansatz ist es, die Dynamik der Elektronen durch eine effektive Temperatur zu modellieren, oder eine Beschreibung im Rahmen kinetischer Methoden. Für die Überpüfung dieser Theorien wurde bisher häufig die modellierte ioneninduzierte Strukturveränderung mit experimentell beobachteten Strukturveränderungen verglichen. Diese "post-mortem" Analysen erlauben es jedoch nicht, Rückschlüsse auf die Kurzzeitdynamik der Elektronen zu ziehen. Um das ioneninduzierte Nichtgleichgewicht der elektronischen Verteilungsfunktion besser zu verstehen, stellen wir im Rahmen dieses Vortrags eine neue Methode vor, welche an die Photolumineszenz-Spektroskopie angelehnt ist. Aus experimentell gemessenen, zeitabhängigen Lumineszenz-Spektren kann die zeitliche Entwicklung der elektronischen Verteilungsfunktion berechnet werden. Umgekehrt lassen sich Lumineszenz-Spektren modellieren, um durch den Vergleich von Experiment und Theorie Rückschlüsse über das ioneninduzierte Nichtgleichgewicht zu ziehen. Diese Modellierung lässt sich mit dem von Rees eingeführten Formalismus [1] effizient durchführen, wie in diesem Vortrag gezeigt wird.

[1] H. D. Rees, J. Phys. Chem. Solids 30, 643 (1969)

DY 17.4 Wed 10:15 ZEU 146

Spin crossover in liquid (Mg,Fe)O from first-principles simulations — •Eero Holmstrom and Lars Stixrude — Department of Earth Sciences, University College London, Gower Street, London WC1E 6BT, UK

When a planet is formed through accretion, it is likely that substantial or complete melting of the body occurs. Understanding the molten state of planetary materials is important, because their solidification sets the initial conditions for the creation and evolution of the lithosphere and atmosphere of planets like the Earth. Using density-functional theory molecular dynamics simulations in conjunction with thermodynamic integration, we model liquid (Mg,Fe)O, the molten phase of the abundant Earth material ferropericlase, at high pressures and temperatures. Firstly, we present a phase diagram of the spin crossover of the Fe ions from a high-spin to a low-spin state with increasing pressure, and predict the equation of state of the melt. Secondly, we compute the electrical conductivity of the liquid. Finally, we assess the implications of our results for the early Earth and other planets.

15 min break

DY 17.5 Wed 10:45 ZEU 146

The fluctuation function of the detrended fluctuation analysis - Investigation of the AR(1) process — •Marc Höll and Holger Kantz — Max-Planck-Institut für Physik komplexer Systeme, Dresden

We derive an analytical expression for the fluctuation function of the first order autoregressive process AR(1) by means of the detrended fluctuation analysis (DFA). This process is short-range correlated and therefore the fluctuation exponent should be $\alpha = \frac{1}{2}$. However the fluctuation function exhibits a crossover between a region with $\alpha > \frac{1}{2}$ and the expected $\frac{1}{2}$. We calculate the crossover point and compare it with the characteristic correlation time of the process.

DY 17.6 Wed 11:00 ZEU 146

Kriging-supported Adaptive Sampling for Non-Oscillatory Central Schemes — •D. G. Roehm[1], R. S. Pavel[2], T. C. Germann[3], and A. L. McPherson[4] — [1]ICP, Universität Stuttgart, Stuttgart, Germany — [2]ECE, University of Delaware, Newark, USA — [3]T1, LANL, Los Alamos, USA — [4]CCS, LANL, Los Alamos, USA

We propose an enhanced adaptive sampling method for heterogeneous multi-scale simulations with stochastic data, based on a non-oscillatory high-resolution scheme for 2D hyperbolic conservation laws. This general framework is used to compute the evolution of a mechanical shock-wave in a perfect copper crystal on the macro-scale by evaluating stress and energy fluxes on the micro-scale. A finite-volume method was used as the macro-scale solver, which launches for every volume element a light-weighted MD simulation (called CoMD) to incorporate details from the micro scale. Since the execution of an MD simulation is rather costly, we reduced the number of actual MD simulations through the use of an adaptive sampling scheme. Our adaptive scheme utilizes a key-value database for ordinary Kriging and a gradient analysis to reduce the number of finer-scale response functions. Kriging estimates an unknown value at a certain location by using weighted averages of the neighboring points. It also provides an error estimate, which we use as trigger for our adaptive scheme. In this contribution we will focus on how the accuracy of the physical values is affected by several thresholds in our adaptive scheme and their connection to the overall performance. The presented adaptive scheme allows for the future inclusion of details present in real materials. (LA-UR-13-29087)

DY 17.7 Wed 11:15 ZEU 146

Optimal model-free prediction of multivariate time series — •Jakob Runge — Potsdam Institute for Climate Impact Research, Potsdam, Germany, and Humboldt University Berlin

We address the problem of predicting a single time series from a set of multivariate predictors in an information theoretic framework. We investigate in how far this can be done optimally given the available information and develop a practical prediction algorithm. The performance and challenges are demonstrated on multivariate nonlinear stochastic delay processes as well as on real data.

DY 17.8 Wed 11:30 ZEU 146

Reconstruction of correlates and construction of surrogates in networked systems — •Annette Witt[1] and Jan Nagler[2] — [1]Max-Planck Institute for Dynamics and Self-Organization and BCCN, Göttingen, Germany — [2]ETH Zürich, Switzerland

Networks with N nodes are considered, each node is associated either to a time series (on the data level) or to its generating stochastic process (on the model level). A link between nodes is represented by a cross correlation functions (ccf), self-loops stand for autocorrelation functions (acf). For the data level we establish conditions for the reconstruction of the complete network from a subnetwork and show that subnetworks which are minimal for reconstruction must connect all N nodes and belong to one of the two network types, namely (i) single-self-loop-trees, where the subnetwork is a tree (i.e. loop-free) with N-1 ccfs and a single acf, and (ii) single-odd-loop-networks, where the given subnetwork consists of N ccfs of which an odd number forms a single loop. For the first time, a parameter-free exact method for the construction of networks on the realization level from networked stochastic processes is given which is employed for generating multi-variate series time with a prescribed cross-spectral matrix. Consequently, the framework is applicable to short- and long-range correlated time series.

DY 18: Granular Matter / Contact Dynamics

Time: Wednesday 9:30–12:45 Location: ZEU 118

DY 18.1 Wed 9:30 ZEU 118

Onset of wall induced convection in vertically oscillated granular systems — •Andrea Fortini — Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, Universitätsstraße 30, D-95447 Bayreuth, Germany

We investigate with two-dimensional computer simulations the onset of the wall-induced convection in vertically shaken granular matter. The convection is one of the major contributing mechanism responsible for the brazil nut effect, i.e. the rise of big particles in a container of small grains. We investigate the convective motion in relation to the dynamical phase diagram of monodispersed grains and show that the wall-induced convection occurs inside the "bouncing bed" region of the parameter space in which the granular bed behaves like a bouncing ball. We find that the onset of the convective motion is caused by the activation of slip mechanisms of the crystalline planes in the closed-packed granular bed. Furthermore, we explore the role of defects and grain boundaries in the onset of convection.

DY 18.2 Wed 9:45 ZEU 118

Emergent surface tension in driven granular media. — •James PD Clewett — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

A liquid-gas-like phase separation is observed in vertically vibrated granular media confined between two horizontal plates. Experiments and simulations were used to show that the coarsening dynamics are spinodal in nature, similar to a system undergoing curvature driven diffusion in the presence of a surface tension (model B). By studying quasi-2d, circular droplets we find behaviour consistent with Laplace's equation. Measurements of the pressure tensor in the interfacial region show that the surface tension is mainly due to an unexpected anisotropy in the kinetic energy components. This is in contrast to equilibrium thermodynamic systems, where surface tension arises due to attractive interactions between particles, or entropic considerations.

DY 18.3 Wed 10:00 ZEU 118

Equilibration of liquid morphologies in granulates with different wettability — •Marc Schaber[1], Mario Scheel[3], Martin Brinkmann[1,2], Marco DiMichiel[3], and Ralf Seemann[1,2] — [1]Experimental Physics, Saarland University, D-66041 Saarbrücken — [2]MPI for Dynamics and Self-Organization, D-37073 Göttingen — [3]European Synchrotron Radiation Facility, F-38000 Grenoble

When adding liquid to dry granulates of spherical beads, the liquid forms individual capillary bridges or a network of liquid morophologies depending on the amount of liquid and the wettability of the granules. Fairly monodisperse glass and basalt microspheres of different diameters are used as granules having small and large contact angle, respectively. By fluidizing the granulate, the packing geometry of the granules is temporarily changed and accordingly the liquid equilibrium distribution is destroyed. Using ultra-fast X-ray tomography we explore the time resolved re-distribution and re-organisation of liquid after stopping the fluidization and the evolution of all the bridges in the granulate. For poorly-wettable basalt beads no liquid redistribution was found. For wettable glass beads, however, a characteristic liquid equilibrium distribution is achieved after a characteristic time scale which depends on bead diameter, the viscosity and the amount of the added liquid.

DY 18.4 Wed 10:15 ZEU 118

Clustering of spinning wet granular hexagons in two dimensions — •Kai Huang and Ingo Rehberg — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

In order to have a more general understanding of the dynamics of wet granular matter, a consideration to the shape of particles is necessary and of practical importance, since spherical particles rarely exist in nature. With a monolayer of vertical agitated wet granular particles with a hexagonal shape, we demonstrate experimentally how the shape of particles influence the collective motion. The particles are covered with a thin liquid film so that short ranged cohesive force may arise from the formation of capillary bridges between adjacent particles. In contast to agitated spherical particles, the hexagonal shaped particles exhibit a strong tendency to spin around its vertical axis, i.e., acting as self-propelled rotors. This type of self-propelled motion is found to hinder the binding of particles through the formation of capillary bridges and hence give rise to dramatically different dynamics towards clustering and crystallization of the particles. The time evolution toward various non-equilibrium steady states of such a granular system and a phase diagram of the steady state with varying agitation parameters and area fractions will be presented.

DY 18.5 Wed 10:30 ZEU 118

Drying in microfluidic cells as a model granular material — •Paolo Fantinel[1,2], Oshri Borgman[3], Ran Holtzman[3], and Lucas Goehring[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August Universität, Göttingen, Germany — [3]Dept. of Soil and Water Sciences, Hebrew University, Rehovot, Israel

We study the drying of porous granular materials on a microscopic scale as to understand macroscopic mechanisms. We aim to develop a 2D pore-scale model through experiments. The long-term goal is to extend such class of models to 3D systems. Ours are microfluidic cells made of an array of pillars,representing the soil grains. The cells are open at one end to allow evaporation. The height is modifiable, as to vary pore elasticity, and we introduce different degrees of heterogeneity by randomly changing particle sizes and positions, as would happen in nature.

We fill the cells with a volatile fluid and watch them dry. At first evaporation happens mainly at the surface, then isolated clusters of fluid form. Through image analysis we find the pressure inside the pores by measuring the curvature of the air-water interfaces. We find a fractal dimension for the liquid-vapor interface of 1.4,close to what expected for percolation. We can also measure the variation in cluster volume, establishing the relative importance of flow through connected pores, thin-film flow and vapor diffusion.

Our experiments are being used together with simulations to establish a micro-scale model of drying in porous media.

DY 18.6 Wed 10:45 ZEU 118

Modeling of a Cohesive, Caking Powder in DEM Simulations — •Alexander Weuster and Dietrich E. Wolf — Uni DuE and CeNIDE, Duisburg, Germany

As the capacity of modern computers increases, it has become feasible to do simulations of bulk solids with particle numbers close to those in real experiments. Capturing every detail, however, remains a challenge, especially when dealing with non-spherical, cohesive particles and a large particle size distribution. Using the the example of μm-sized potassium chloride (KCl), we will present an approach to model

a cohesive, caking powder in DEM-Simulations. By calibration of an idealized ensemble of spheres, we are able to reproduce the macroscopic flow properties of KCl observed in experiments.

15 min break

DY 18.7 Wed 11:15 ZEU 118

Observation of homogeneous crystallization in sphere packings — •Frank Rietz[1], Charles Radin[2], Harry L. Swinney[3], and Matthias Schröter[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — [2]University of Texas at Austin, Department of Mathematics — [3]University of Texas at Austin, Center for Nonlinear Dynamics

Sphere packings serve as a model for the microscopic structure of matter. Similar to atoms, spheres arrange in disordered and ordered phases. The densest disordered packing that is achievable for many experimental protocols is known as Random Close Packing. Frustration inhibits further increase of the density by crystallization. The theoretical picture of this barrier is still unclear.

In our experiment the sphere packing is driven by periodical tilting of the container side walls. Three-dimensional information is obtained by an index matching technique [1]. The initial disordered packing compacts and above the Random Close Packing density we observe homogenous crystallization of the interior spheres. We characterize this first order phase transition by measurement of local volumes, crystal growth rates and critical nucleus size. Investigation of local structural changes allows us to better understand the jamming at the Random Close Packing density.

[1] J. A. Dijksman et al., Rev. Sci. Instrum. 83, 011301 (2012).

DY 18.8 Wed 11:30 ZEU 118

Nearly-2D granular packings: A mechanical analogue to frustration in spin systems — •Kirsten Harth[1], Alexander Mauney[2], Frank Rietz[1], and Ralf Stannarius[1] — [1]Institut für Experimentelle Physik, Otto von Guericke Universität Magdeburg, Germany — [2]North Carolina State University, Raleigh, USA

Frustration of antiferromagnetic spins on a triangular lattice represents a fundamental problem in theoretical studies of magnetism, and is usually not experimentally observable on the microscale. Recently, an analogous problem has been investigated on an easily accessible length scale, using colloidal particles in a horizontal cell [1].

In granular materials, similar structures are easily prepared with glass spheres in a quasi-2D vertical cell, the cell thickness being slightly larger than the particle diameter. In nearly-hexagonal packings, some of the spheres attach to the front plate while others attach to the rear plate. By mapping the positions of the glass spheres experimentally, statistics of the degree of frustration are performed. Additionally, the influence of a magnetic field on the frustration statistics is mimicked by tilting the cell with respect to the normal in the gravitation field at well-defined angles, such that rear particles are energetically favoured.

[1] Y. Han, Y. Shokef, A. M. Alsayed, P. Yunker, T. C. Lubensky, Nature 7595, p. 898 (2008)

DY 18.9 Wed 11:45 ZEU 118

Ordering of Vertically Agitated Granular Rods in a Circular Confinement — •Thomas Müller, Ingo Rehberg, and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

Agitated granular matter can be considered as a non-equilibrium mode system for phase transitions and pattern formation. From this perspective, spherical particles have been frequently investigated in the past. However, in plenty of natural systems or industrial applications, one also has to deal with anisotropic particles like rice, medicine capsules, wood pellets etc.

Due to their anisotropy, granular rods share many properties with the well investigated rod-like liquid crystals, such as a transition from an isotropic to a nematic ordering phase. Although thermal energy can effectively mix liquid crystal molecules, continuous energy injection is needed for the self-organization of granular particles to compensate the energy dissipation. Under agitation, such dissipative systems can then evolve into ordered states or distinct patterns.

We study a single layer of monodisperse granular rods in a circular cavity which is vertically driven at various amplitude and frequency. By varying the packing fraction and the aspect ratio of the rods, we experimentally explore different orientational ordering phases and also compare with computer simulations.

DY 18.10 Wed 12:00 ZEU 118

MC-Simulation of Packings of Regular Tetrahedra — •Lukas Zwirner and Eckard Specht — Otto-von-Guericke Universität Magdeburg, Institut für Experimentelle Physik/Materialphysik

The problem of packing tetrahedra attracted much interest recently. For regular tetrahedra the densest known packing has a packing fraction of $\phi \approx 0.8563$. It is a periodic packing of double dimers (Chen et al., Discrete Comput. Geom. 44, p. 253 (2010)).

However, searching for a high packing fraction is not the only topic of interest, e. g. the wide field of quasi-crystals or behavior of granular matter are subject of current research.

We investigate the problem of packing identical, regular tetrahedra numerically by a pure geometrical approach. Hence, there is neither friction nor torques. The Monte-Carlo-method is applied to generate packings of regular tetrahedra using different protocols.

The packings are investigated with regard to their spatial structure (pair correlation function), their pairwise orientation and face-normal correlation.

DY 18.11 Wed 12:15 ZEU 118

Simulation of Current-Activated Pressure-Assisted Densification — •Sebastian Angst and Dietrich E. Wolf — Physik, Universität Duisurg-Essen

Cohesive particles usually form very porous agglomerates. They support loads up to a consolidation pressure, which increases with decreasing particle size. Compaction of nano-powders can therefore be very costly and time consuming. If the particles are electrically conducting, which is the case e.g. for novel nano-structured thermoelectric materials, the technique of current-activated pressure-assisted densification (CAPAD) turns out to have many advantages. Electrical power deposited locally as Joule heat lowers the consolidation pressure such that higher densities without much coarsening are obtained. We present a new model combining particle dynamics, calculated by molecular dynamic methods, with a network model including thermoelectric properties.

DY 18.12 Wed 12:30 ZEU 118

Self-Assembly of Spherical Magnets — •Igor Stanković[1], Lara Abou Khali[2], and René Messina[2] — [1]Scientifc Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [2]Institut de Chimie, Physique et Materiaux (ICPM), Universite de Lorraine, 1 Bd. Arago, 57070 Metz, France

The self-assembly of spherical magnets is addressed theoretically. Minimal energy structures are obtained by optimization procedures as well as Monte Carlo computer simulations. Three typical shapes are obtained depending on the number of constitutive magnets N. In the regime of small N, chains are stable as dimers or trimers (i.e., $N \leq 3$), then rings become stable for ($4 \leq N \leq 13$) where dipole vectors adopt a vortex-like arrangement. A major finding concerns the stacking of rings as soon as N is large enough ($N \leq 14$). All the relevant predicted shapes are experimentally reproduced by manipulating commercial magnets.

DY 19: Energy Meets Economy: Dynamics and Statistics of Future Energy Systems (joint session SOE/DY/ jDPG)

Time: Wednesday 11:45–13:15 Location: GÖR 226

DY 19.1 Wed 11:45 GÖR 226

Fluctuation analysis of high frequency electricity power load in the Czech Republic — •Hynek Lavicka[1,2] and Jiri Kracik[3] — [1]Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Physics, Břehová 7, CZ-11519 Praha 1, Czech Republic — [2]Bogolyubov Laboratory of Theoretical Physics, Joint Institute of Nuclear Research, RU-141980 Dubna, Russia — [3]Charles University in Prague, Faculty of Social Sciences, Institute of Economic Studies, Opletalova 26. CZ-110 00 Prague 1, Czech Republic

We focus our analysis on data of electricity power loads in Czech Republic which exhibits seasonality and well as periodic trends typical for other European states. We separate the signal into two parts in Fourier picture where the data undergo power law with significant peaks. Deterministic part governs seasonal and periodic trends. While the latter part holds information on random fluctuations. To deeply analyze stochastic part we employ Multifractal Detrended Fluctuation Analysis (MF-DFA) to determine estimation of Hurst exponent and scaling exponent. Power law exponent of MF-DFA depends on parameter of analysis for stochastic and shuffled stochastic part. This behavior is typical for heavy-tailed distributions. Moreover we also determined properties of autocorrelation function and we found long-range correlation which depends on parameter of analysis.

DY 19.2 Wed 12:00 GÖR 226

Large-deviation properties of power grids — •Timo Dewenter and Alexander K. Hartmann — Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg

We study numerically a Kuramoto-like model [1,2] on different standard and spatial random graphs, which is used to describe the dynamical behavior of coupled mechanical rotators. Such a turbine is represented by a node in the graph, whereas edges stand for transmission lines which can transmit power up to a maximum capacity P^{MAX} between the machines. A machine can either produce (generator) or consume (motor) power. Here, we investigate the robustness of such networks of the random graph ensemble against transmission line failures, i.e. removal of edges. The measured histograms of the robustness certainly provide only information for the smallest probabilities being of order $1/N_{\mathrm{samp}}$, where N_{samp} is the number of samples used to generate the random graph ensemble. Therefore, we apply a large-deviation approach [3] to obtain the low-probability tails of the distribution, which allows us to gain insight in the topology of extreme robust and extreme vulnerable networks.

[1] G. Filatrella, A.H. Nielsen, N.F. Pedersen, Eur. Phys. J. B **61**, 485 (2008)
[2] M. Rohden, A. Sorge, M. Timme, D. Witthaut, PRL **109**, 064101 (2012)
[3] A.K. Hartmann, Eur. Phys. J. B **84**, 627 (2011)

DY 19.3 Wed 12:15 GÖR 226

Extending electric grid physics to implement smart grid trading function — •Thomas Walter and Bernd Brunner — Wirsol Integrated PV Solutions

Renewable energy (RE) sources like solar and wind can now compete on generation cost with some fossil sources, but have the property of being volatile. Traditional concepts use storage of electric energy to compensate for this volatility. However, storage cost exceeds generation cost until major breakthroughs will be achieved. Electric grids in which reneable energies provide the larger share (RE dominated grids) therefore utilize the flexibility of decentral loads and generation units. If these are shifted suitably in time, they can utilize too high RE production, and supply energy when RE production is too low. The paper shows how the well known effect that grid freguency varies according to the balance of supply and demand can be utilized to build the basis of a smart grid. This system simplifies overall complexity and reduces cost by appropriate combination of physics and data based technologies.

DY 19.4 Wed 12:30 GÖR 226

Imaginary Interest Rates and Complex Net Present Value Calculus in Energy Economics — •Gunnar Kaestle — Clausthal University of Technology, 38678 Clausthal-Zellerfeld, DE

A helpful instrument for evaluating the economic feasibility by integrating cash-flows is the Laplace transform [1], as it is an equivalent for net present value calculation. Mathematic rules known from control theory are able to simplify economic assessments. Introducing interest rates from the two-dimensional plane of comlex numbers expands their descriptive power from purely growth or decline to cyclical processes.

Besides discounting cash-flows, discounting energy flows is also a more general but very important assessment of investments in the energy sector. The limiting EROI-factor is gradually degrading in the fossil fuel sector due to the human nature to go for the low hanging fruits first. Severe long term economic implications have to be anticipated, due to the fact that energy is a very powerful production factor.

Therefore, a controlled transition towards non-exhaustive energy resources with a stable EROI has to be started when discretionary spending in learning investments and the deployment of new technology is still possible. The so called net energy cliff shall be avoided by following an exergy efficient transition pathway. Incentive schemes such as the self-adjusting feed-in tariff for German PV systems can be interpreted as supervisory economic control loops.

[1] Robert Grubbström: On the Application of the Laplace Transfrom to Certain Economic Problems; Management Science; Vol. 13; No. 7; 1967; pp. 558-567.

DY 19.5 Wed 12:45 GÖR 226

Self-Organized Synchronization and Voltage Stability in Power Grids Modeled by Networks of Synchronous Machines — •Katrin Schmietendorf[1], Joachim Peinke[1], Oliver Kamps[2], and Rudolf Friedrich[3] — [1]Carl von Ossietzky Universität Oldenburg, Institut für Physik, ForWind — [2]CeNoS, Münster — [3]WWU Münster, Institut für Theoretische Physik

The energy transition is accompanied by grid decentralization and fluctuating power feed-in characteristics. Hence, with a view to future grids, power system stability and design are actual key issues.

We investigate power system stability in terms of self-organized synchronization aspects on the basis of a network of coupled synchronous machines. In recent years, a relationship between this approach and synchronization phenomena described by the well-known Kuramoto model (KM) has been uncovered. The KM models the dynamical behaviour of coupled oscillators displaying a phase transition from incoherent to partially synchronized states at a critical coupling value. In contrast to other attempts, our network model incorporates both rotor angle and voltage dynamics plus the feature of angle-voltage stability interplay. It can be shown to correspond to a novel version of the KM with time-varying coupling coefficients, which has not been investigated in the context of nonlinear dynamics yet.

We discuss the model's potential applications to modern power systems with a high percentage of renewable energy plants and present results concerning the stability properties of small two-machine units up to large networks.

DY 19.6 Wed 13:00 GÖR 226

Power transmission in a renewable European future — •Sarah Becker[1], Rolando Rodriguez[2], Martin Greiner[2], and Stefan Schramm[1] — [1]FIAS Uni Frankfurt, Germany — [2]Uni Aarhus, Denmark

We investigate a renewable-based European electricity system, where wind and solar PV produce as much energy as is consumed. Since this generation flucuates with the weather, there will in general be a mismatch between load and generation in individual hours. We assume deficits to be covered by dispatchable power plants, while excesses are curtailed.

In this setting, we study different flow paradigms for inter-country power transmission, i.e. ways to share renewables and match deficits and excesses between the countries. Particular focus is placed on the effects on backup energy usage ("how much fuel is burned?"), backup capacity needs ("how many dispatchable plants need to be available?"), and transmission line investments. Furthermore, we examine different approaches to transmission grid strengthening and compare actual and optimized developments.

DY 20: Focus Session: Modelling of Non-linear Dynamics in Biological Movement (joint session BP/ DY)

Time: Wednesday 14:00–16:30 Location: ZEU 250

Topical Talk DY 20.1 Wed 14:00 ZEU 250

Legged locomotion. - From biology to mechanics and return. — •Reinhard Blickhan — Science of Motion, Jena, Germany

The locomotory system of animals has to cope with external and internal physical conditions confining and shaping the evolutionary space. This space can be probed by combining experimental observations with modelling supported by numerical simulations. To sustain locomotion animals are enforced to use oscillatory modes. In terrestrial locomotion this led to the development of legs in arthropods and vertebrates. Physical suitability combined with the requirement to enhance power and/or efficiency and to reduce or facilitate the control effort shape the space of solutions. We can show that gaits such as bipedal walking, grounded running, and running do represent an outcome of a compliant system being operated under different initial conditions. As nonlinear systems these systems inherit the property of attractive modes of operation which are used to reduce the control effort. During locomotion the legs as structural elements must fulfil their prescribed task efficiently. Segmentation of legs must prove itself with respect to this demand. The muscle as a common actuator is traded through evolution. Nevertheless, we start to understand that muscles seem to aggregate properties such as compliance, damping, and a geared output in a rather suitable and adaptable way. An integrative view covering the different levels of organization and the vast range of designs may help us to deduce general principles.

DY 20.2 Wed 14:30 ZEU 250

Learning Motor Skills with Information-Theoretic Approaches — •Jan Peters[1,2], Christian Daniel[1], and Gerhard Neumann[1] — [1]Technische Universität Darmstadt — [2]Max Planck Institut für Intelligente Systeme

Synthesizing new motor skills from data has been a long standing vision of robotics, artificial intelligence, and the cognitive sciences. A first step towards this goal is to create approaches that can learn tasks triggered by environmental context or higher level instruction. However, learning techniques have yet to live up to this promise as only few methods manage to scale to high-dimensionality of humans and anthropomorphic robots. In this talk, we investigate a general framework suitable for learning motor skills in robotics and for explaining human movement learning which is based on the information-theoretic principles, such as movement organization, representation and acquisition by information entropy. As a result, the framework involves generating a representation of motor skills by parameterized motor primitive policies acting as building blocks of movement generation, and a learned task execution module that transforms these movements into motor commands. We discuss task-appropriate information-theoretic learning approaches for movements and illustrate their effectiveness on human movement data and in robot motor skill learning on both toy examples (e.g., paddling a ball, ball-in-a-cup) and on playing robot table tennis.

DY 20.3 Wed 14:45 ZEU 250

Humans run like pogosticks - with ankles — •Horst-Moritz Maus[1], Shai Revzen[2], John Guckenheimer[3], Christian Ludwig[1], Johann Reger[4], and Andre Seyfarth[1] — [1]TU Darmstadt, Deutschland — [2]University of Michigan, Ann Arbor, USA — [3]Cornell University, Ithaca, USA — [4]TU Ilmenau, Deutschland

Running is an essential mode of human locomotion. Its large number of biomechanical and neural degrees of freedom are often modeled as a simple Spring Loaded Inverted Pendulum (SLIP). The SLIP body bounces as if on a pogo stick, pivoting on its spring leg and then jumping through a ballistic aerial phase. Updating SLIP model parameters to fit each step can result in trajectories that follow an observed path much more closely. These parameter updates represent a control input modulating the uncontrolled SLIP dynamics to obtain human-like movement and stability. Here we systematically construct a minimalistic *ankle-SLIP* model from measurements of humans running on a treadmill. Using Data Driven Floquet Analysis we identify candidate predictors for the parameter changes. Selecting a predictor related to ankle state allows us to predict running motion stride to stride and mimic rates of recovery from perturbation. We reveal inherent limitations in predictions made by other SLIP variants. Our methods produce a systematic means to search for prediction enhancing, yet low dimensional models of rhythmic processes in the physical sciences. More directly the "ankle-SLIP" models may impact gait assessment in sports and in clinical contexts and suggest control strategies for humanoid robots and prosthetic limbs.

DY 20.4 Wed 15:00 ZEU 250

Quantifying control effort of biological and technical movements: an information entropy based approach — •Daniel Häufle[1,2], Michael Günther[1], Günter Wunner[2], and Syn Schmitt[1,3] — [1]Institut für Sport- und Bewegungswissenschaft, Universität Stuttgart, Germany — [2]Institut für Theoretische Physik 1, Universität Stuttgart, Germany — [3]Stuttgart Research Centre for Simulation Technology, Universität Stuttgart, Germany

In biomechanics and biorobotics muscles are often associated with reduced movement control effort compared to technical actuators. This is based on the notion that the muscle properties positively influence movement control and allow for simpler controllers. Other physical measures, such as energy consumption, stability, or jerk, have already be applied to compare such systems. However, previous definitions of control effort were based on system specific measures, such as voltages, forces, muscle activity, etc., which made it impossible to quantitatively compare the control effort of different actuation systems. Here, a system independent measure of control effort based on information entropy is presented. By calculating the Shannon information entropy of all sensor signals required for control, models of biological and technical control systems can be compared. Exemplarily applied to (biomechanical) models of hopping it reveals that the required information for controlling hopping is only $I = 32$bit with a muscle vs. $I = 660$bit with a DC-motor. This approach to control effort is thus applicable to and comparable across completely different actuators and control approaches.

DY 20.5 Wed 15:15 ZEU 250

COMPUTATIONAL MODEL FOR A FLEXIBLE SENSORIMOTOR MEMORY BASED ON A RECURRENT NEURAL NETWORK — •Kim Joris Boström and Heiko Wagner — Motion Science, University of Münster, Germany

The motor system has the unique capacity to learn complex movements in a flexible manner. Using recent recurrent network architecture based on the reservoir computing approach, we propose a computational model of a flexible sensorimotor memory for the storage of motor commands and sensory feedback into the synaptic weights of a neural network. The stored patterns can be retrieved, modulated, interpolated, and extrapolated by simple static commands. The network is trained in a manner that corresponds to a realistic exercising scenario, with experimentally measured muscular activations and with kinetic data representing proprioceptive feedback. The model may help to explain how complex movement patterns can be learned and then executed in a fluent and flexible manner without the need for detailed attention. Furthermore, it may help to understand the reafference principle in a new way, as an internal feedforward model for the prediction of expected sensory reafference would no longer be necessary. Instead, the reafference would be learned together with the motor commands by one and the same network, so that neural resources were exploited in a highly efficient way.

DY 20.6 Wed 15:30 ZEU 250

A COMPUTATIONAL MODEL EXPLAINS THE RELATIONSHIP BETWEEN MUSCULAR CO-ACTIVATION, REFLEXIVE CONTROL AND SELF-STABILITY — •Heiko Wagner and Kim Joris Boström — Motion Science, University of Münster, Germany

Sustaining stability during bipedal locomotion poses a challenge to the neuro-muscular-skeletal system, not only for the extremities but also for the spine. Commonly, a major role in maintaining stability is attributed to the reflex control system, which, however, is limited by the neural conduction velocity. For this reason, the concept of self-stability has been introduced, which claims that the mechanical properties of the muscular-skeletal system are exploited to maintain stability via muscular co-activation. Based on a computational model,

we analyze the relationship between muscular co-activation, reflexive control and self-stability. The model includes pelvis, rib cage, and lumbar spine, as well as 90 Hill-type muscles, each endowed with a delayed monosynaptic reflex based on the lambda model. We show that muscular co-contraction not always increases the stability of the system, but rather that for a given reflex delay time there exists an optimal amount of co-contraction. These results may have an impact on the understanding of the motor control system in general, and in particular of the pathological reflex delay found in patients with low back pain.

DY 20.7 Wed 15:45 ZEU 250

How to turn the non-linear muscle into a linear all-purpose tool — •Karl Theodor Kalveram — Heinrich Heine Universität Düsseldorf, Germany — Technische Universität Darmstadt, Germany

The three basic categories of biologically motivated tasks that we discriminate we call "reaching", "cycling" and "enforcing". Because in all these activities the physical environment has to be influenced in a scaled manner, the organism must provide appropriately scaled forces. Our muscular-skeletal system solves those problems. We ascribe this to the organism's property to generate forces by muscular activation, and to generate this activation through neural stimulation. It remains, however, the open question, how to specify that stimulation, which exactly produces that forces, which are necessary to complete the respective task correctly?

Here we propose a control schema, which makes the non-linear Hill-type muscle a multiple-purpose tool for solving the biologically imposed motor tasks mentioned above. We achieve this by training an artificial neural network by a two-step auto-imitative learning algorithm (a special type of learning by regression), which makes the network an adaptive inverse controller of the physical environment to be controlled.

DY 20.8 Wed 16:00 ZEU 250

Computer simulation in biomechanics – past, present, future — •Hanns Ruder[1] and Syn Schmitt[2] — [1]Theoretische Astrophysik, Universität Tübingen — [2]Human Movement Simulation Lab, Universität Stuttgart

Since the beginning of science, humans wonder about, observe, and try to understand Nature. They do so by using the available tools and methods of their time to the best of their knowledge. In classical physics, over a century ago, research on the phenomena of life was common and driven by the desire to test the universality of physical laws. Already in 1906, Otto Fischer published theoretical considerations on studying the mechanics of human movement. Later, with the invention of computers, numerics helped researchers to solve more complex problems. It is now possible to study the birth and death of stars and the history of our universe. These new possibilities that come with Simulation technology are said to be the scientific paradigm of our age encouraging researchers from all disciplines to use these new methods. As physicists, we use reduced models to explore Nature and, for example in biomechanics, seek principles of human movement. We share the understanding that the very same forces which move the stars in the universe move the hips to let humans walk. Thus, computer simulations can help to understand the phenomena of human movement.

In this talk, we will discuss the organisation of biological material fulfilling the known principles of physics to walk, run, or jump. In short: from wobbling masses to intervertebral discs.

DY 21: Pattern Formation

Time: Wednesday 15:00–18:00 Location: HÜL 186

DY 21.1 Wed 15:00 HÜL 186

Pattern selection in liquid crystal growth — •Martin von Kurnatowski and Klaus Kassner — Otto-von-Guericke-University Magdeburg, Department of Theoretical Physics, Universitätsplatz 2, 39106 Magdeburg

The interface of a smectic liquid crystal growing in its undercooled nematic phase forms dendritic patterns. The problem can be described by a simple symmetric diffusion model. In the case of liquid crystals heat transport is anisotropic. However, anisotropic surface tension is required to stabilize the pattern and determine its length scale. The growth is faster in the direction of less efficient heat transport ("inverted growth"). Any physical solution should include this feature.

The solution is derived from an expansion about the case without capillary effects. Including anisotropic surface tension yields an eigenvalue problem for the growth mode. We solve this selection problem of dendritic growth in anisotropic diffusion using the method presented by us in [1]. The length scale is predicted and a quantitative description of the inverted growth phenomenon is given.

[1] M. von Kurnatowski et al., Phys. Rev. E 87 042405 (2013)

DY 21.2 Wed 15:15 HÜL 186

Orientational selection in pattern formation by traveling modulations — •Lisa Rapp[1], Vanessa Weith[1], Alexei Krekhov[1,2], and Walter Zimmermann[1] — [1]Theoretische Physik, 95440 Universität Bayreuth, Germany — [2]Max-Planck-Institut für Dynamik und Selbstorganisation, 37077 Göttingen, Germany

Often disordered stripe patterns occur in two-dimensional isotropic systems, such as in reaction diffusion systems, in thermal convection or in block copolymers. We suggest an effective approach to control the pattern morphology by applying a traveling long-wave periodic modulation of the control parameter of the pattern forming system. The model systems we investigate include the Swift-Hohenberg, the evolution equation for microphase separation in symmetric diblock copolymers and the Lengyel-Epstein model for chemical reactions. Studying the onset of the stripe phase we find that depending on the traveling velocity v different orientations of the stripes with respect to the modulation may be favoured near threshold. In case of a stationary modulation the wave vector of the stripes is preferentially perpendicular to the wave vector of the forcing. This also holds for velocities smaller than a velocity v1. For velocities larger than a velocity v2 a parallel orientation of the wave vectors has the lowest threshold. In the intermediate range $v1 < v < v2$ both wave vectors adjust themselves at an angle between 0 and $\pi/2$.

DY 21.3 Wed 15:30 HÜL 186

The two-dimensional Kuramoto-Sivashinky equation generalized by a linear and a quadratic damping term — •Marc Osthues, Christian Diddens, and Stefan J. Linz — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster

Inspired by the effect of particle redeposition in the context of self-organized pattern formation on ion-beam eroded semiconductor targets [1,2], we investigate a generalization of the two-dimensional Kuramoto-Sivashinky equation by additionally considering a linear and a quadratic damping/stabilization term. The analysis of the resulting equation by numerical simulations, amplitude equations and Galerkin approximations reveals a variety of solution types depending on the entering parameters. The arising morphologies range from spatio-temporal chaotic dynamics and blinking states to hexagonally arranged dot and hole patterns as well as ripple structures [3].

[1] C. Diddens and S. J. Linz, EPL, 104 (2013) 17010
[2] C. Diddens and S. J. Linz, Eur. Phys. J. B, 86 (2013) 397
[3] M. Osthues, C. Diddens and S. J. Linz, (in preparation)

DY 21.4 Wed 15:45 HÜL 186

Collective behaviour of shifted dipoles in external fields — •Arzu Bahar Yener and Sabine H. L. Klapp — Hardenbergstr. 36, 10623 Berlin, Germany

A colloidal system of spherical particles with centred dipolar mo- ments show self-organisation to layered structures in the presence of an external rotating magnetic field [1]. This non-equilibrium phenomenon requires synchronised motion of the particles with each other and with the driving field [1].

We investigate a model system of spherical particles carrying permament dipole moments shifted out of the centres of mass and interacting by a soft core potential and a point dipole potential. Such system can be used to model experimentally created particles with magnetic caps [2] or Janus particles [3]. We aim to describe the non-equilibrium behaviour of the system in external rotating magnetic fields, using molec-

ular dynamics simulations. We present groundstate structures of the shifted dipolar system as well as simulation results in the presence or absence of external magnetic fields. [1] S. Jäger, and S. H. L. Klapp, Soft Matter 7, 6606 (2011) [2] D. Zerrouki, J. Baudry, D. Pine, P. Chaikin, and J. Bibette, Nature 455, 380 (2008) [3] J. Yan, M. Bloom, S. C. Bae, E. Luijten, and S. Granick, Nature 491, 578 (2012)

DY 21.5 Wed 16:00 HÜL 186

Phase separation by Marangoni flow drives active droplet — •Max Schmitt and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

One possible design of a spherical microswimmer is a water droplet in an oil phase with surfactants at the interface [1]. Bromine inside the droplets catalyzes a reaction, which saturates the double bond in the surfactant molecule, making it a weaker surfactant with a higher surface tension. The resulting binary mixture of surfactants will then demix due to Marangoni flow, initiated by and directed along a surface tension gradient. Thus a so-called squirmer results, which reaches a steady swimming state, when the surface is covered with only two domains that cannot demix any further.

We have extended our recently developed model based on a reaction-advection-diffusion equation for the surfactant mixture on an axisymmetric sphere [2], by considering a sphere without axisymmetry and by adding thermal noise. This allows us to trace back the random walk of the squirmer visible in its swimming trajectory to local fluctuations in the surfactant mixture. Furthermore, we investigate the time-dependence of the coarsening dynamics of the surfactant mixture and compare it to results from the classical Cahn-Hilliard theory for phase separation.

[1] Thutupalli S. *et al New J. Phys.* **13** 073021 (2011)
[2] Schmitt M. and Stark H., *Europhys. Lett.* **101** 44008 (2013)

DY 21.6 Wed 16:15 HÜL 186

Pattern formation in anisotropic systems with modulation: stripes versus defects — •Badr Kaoui, Achim Guckenberger, Falko Ziebert, Alexei Krekhov, and Walter Zimmermann — Theoretical Physics I, University of Bayreuth, 95440 Bayreuth, Germany

A new symmetry class of pattern formation is investigated, having an anisotropy direction and a modulation perpendicular to the former. An example for this situations is the wrinkle pattern that forms during the relaxation of a deposited thin solid film (e.g. oxide) on a stretched soft substrate (e.g. a PDMS elastomer). If the substrate elastic properties are anisotropic perpendicular to the direction of prestretching, beyond a critical modulation strength, a fascinating competition occurs between the emergence of perfect regular stripes and wrinkles including branching defects. Using pseudo-spectral simulations and linear stability analysis we show how spatial modulations induce a wave-number band of patterns including various defect orders. We found unexpectedly the existence of a band of stable defect free stripe patterns and we predicted when and how these stripes bifurcate from the defect and flat ground states. Related universal phase diagrams are drawn with possible applications to the wrinkles system and the dissipative counterpart of the electroconvection in nematic liquid crystals.

15 min break

DY 21.7 Wed 16:45 HÜL 186

Mode transitions of oscillating water drops — •Frank Rietz and Stefan C. Müller — University of Magdeburg, Institute of Experimental Physics, Pattern Formation Group

Drop oscillations occur, for example, in the rain and play a role in technological processes. The process by which a pollutant is incorporated into a rain drop depends on its shape, which changes drastically during the oscillation. Such oscillations are easily observed, if water is poured on a hot plate. At sufficiently high plate temperature the drop floats on its own steam film. The thin sheet thermally insulates the liquid and the drop survives for several minutes (Leidenfrost-effect). During the evaporation process the drop oscillates in different eigenmodes that resemble star-like shapes. The modes of the star-shaped drops spontaneously change in irregular periods. For evaporating drops on a hot plate we measure the relation between mode change, drop size, and oscillation period. Experiments are performed at shrinking and constant drop volume.

DY 21.8 Wed 17:00 HÜL 186

Cracking over patterned substrates — •Pawan Nandakishore, Anupam Sengupta, and Lucas Goehring — Max Planck Institute for Dynamics and Self-Organization (MPIDS) 37077 Göttingen, Germany

From thermal cracks on the surface of Mars to desiccation cracks in dried paint, cracking occurs at all length scales. In the above examples the substrate structure influences the resulting crack pattern. We study the effect of the substrate by generating desiccation cracks on patterned substrates over various length scales. On the macro (decimeter) scale, we dry Bentonite slurries over sinusoidal substrates and study them using time lapse photography. The wavelength, amplitude of the substrate and the layer height of the clay are the relevant parameters. We use an orientational order parameter to characterize the crack pattern. We find that the order parameter evolves non-monotonically with layer height which hints that when the layer height is comparable to the wavelength there is roughly a crack on top of every peak, such a pattern is characterized by a high order parameter. We fabricate sinusoidal substrates on the micro scale by oxidizing thin films of PDMS under strain. We deposit Bentonite, laponite and other colloidal suspensions on the patterned PDMS substrates and study their drying and cracking behavior. Combining observations at both length scales we attempt to decipher what lies beneath a crack pattern.

DY 21.9 Wed 17:15 HÜL 186

Roles of pattern competition in diversity-induced resonance — •Miriam Grace and Marc-Thorsten Hütt — Jacobs University Bremen, Bremen, Germany

The phenomenon of diversity-induced resonance, in which a system's response is enhanced at intermediate parameter disorder, has been studied for several years in wide-ranging contexts. We previously used an event-based view to understand developmental paths to spatiotemporal patterns [1,2]. We here explore the mechanisms of diversity-induced resonance in FitzHugh-Nagumo lattices, analyzing the competitive interactions between spiral and target wave events subject to differing levels of diversity [3]. We use minimal-ingredient lattices to understand how the diversity parameters control aspects of these competition scenarios. This form of diversity-induced resonance arises from different types of pattern competition: frequency-based interactions of target and spiral waves, and competition determined by the properties of parameter distributions. The resonance responses of wave counts to diversity are statistically controlled by the number of oscillatory elements in the lattice, rather than by the frequency differences between target and spiral waves.

1. Geberth, D. and Hütt, M.-Th (2009) PloS Comput. Biol. 5, doi: 10.1371/journal.pcbi.1000422
2. Grace, M. and Hütt, M.-Th. (2013). J. R. Soc. Interface 10, doi: 10.1098/rsif.2012.1016.
3. Grace, M. and Hütt, M.-Th (submitted). Eur. Phys. J. B.

Invited Talk DY 21.10 Wed 17:30 HÜL 186

Episodic Precipitation — •Jürgen Vollmer — Max Planck Institute for Dynamics and Self-Organization (MPI DS), 37077 Göttingen, Germany — Faculty of Physics, Georg August University, 37077 Göttingen, Germany

Episodic outbreaks with potentially catastrophic consequences are characteristic of geysers, as well as lake, oceanic and volcano eruptions. These processes have in common that a slow continuous mass or heat flux into a fluid mixture leads to slow bubble growth, and that episodically the material accumulated in the bubbles is released in explosive precipitation events. The slow growth of the bubbles in response to the flux involves phase separation and ripening. Indeed, periodic modulations of precipitation rates arise also in laboratory experiments where phase separation in binary fluids is monitored during a temperature ramp.

To gain insight into the origin of this episodic precipitation, I revisit the evolution of the droplet size distribution. The net flux to the droplets constitutes an essential perturbation to the Lifshitz-Slezov-Wagner scenario of zero flux. Any finite flux leads to qualitatively different growth laws. Accounting for these differences, I provide a quantitative description of the time scale, Δt, separating subsequent outbreaks in our experiments.

DY 22: Statistical Physics (general)

Time: Wednesday 15:00–18:15 Location: ZEU 160

DY 22.1 Wed 15:00 ZEU 160

Hamiltonian adaptive resolution simulations of soft matter — •Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz

Many phenomena occurring in soft matter, from the interaction of biomolecules to the self-assembly of biological as well as artificial nanocomposites, cover a broad range of length and time scales. Being hardly amenable with a fully-atomistic approach, these systems are usually addressed with multiscale simulation methods, aimed at building computationally efficient coarse-grained models that, in many cases, suffer the lack of important chemical details. To circumvent this problem, adaptive dual-resolution schemes have been developed to concurrently use different levels of resolution in different regions of the same system, yet allowing molecules to freely diffuse across the simulation domain. Here a method is presented, the Hamiltonian Adaptive Resolution Simulation (H-AdResS) scheme, which, in contrast to previous approaches, is built in terms of a Hamiltonian function; this makes it possible to formulate a solid statistical physics theory of dual-resolution systems and, as a consequence, it allows one to use the preferred statistical ensemble as well as the simulation algorithm. Applications of H-AdResS will be discussed, such as microcanonical simulations of simple molecular fluids and Monte Carlo simulations of mixtures.

DY 22.2 Wed 15:15 ZEU 160

parQ - Infinite Temperature Transition Matrix Monte Carlo in the Canonical and Grand Canonical Ensemble — •René Haber and Karl Heinz Hoffmann — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

We investigate properties of our transition matrix Monte Carlo method par$Q$[1] in the canonical and grand canonical ensemble. It estimates the transition probabilities at infinite temperature in a given macrostate range by counting all proposed transitions during a simulation. At the end of the simulation the eigenvector corresponding to the eigenvalue 1 is calculated, which can be identified as the density of states. The method is easily parallelizable and can be combined with different sampling schemes like standard Metropolis sampling, Wang-Landau sampling as well as transition matrix Monte Carlo. The influence of different sampling schemes and different eigenvector solving algorithms is presented.

[1] F. Heilmann and K. H. Hoffmann. Europhysics Letters, 70(2):155-161, 2005.

DY 22.3 Wed 15:30 ZEU 160

Dynamics in Stochastic Optimization: Combining Stochastic Tunneling and Energy Landscape Paving — •Kay Hamacher — Depts. of Physics, Computer Science, and Biology, TU Darmstadt

Heuristic optimization schemes such as simulated annealing, genetic algorithms, or extremal optimization play a most prominent role in global optimization. The performance of these algorithms and their respective sampling behavior during the search process are themselves interesting problems - in particular from the viewpoint of dynamical systems theory and statistical mechanics.

Here, we show that a combination of two approaches * namely Energy Landscape Paving (ELP) and Stochastic Tunneling (STUN) * can overcome known problems of other Metropolis-sampling-based procedures. We show on grounds of non-equilibrium statistical mechanics and empirical evidence on the synergistic advantages of this combined approach and discuss simulations for a complex optimization problem.

Reference: [1] K. Hamacher. A New Hybrid Metaheuristic - Combining Stochastic Tunneling and Energy Landscape Paving, 8th International Workshop on Hybrid Metaheuristics (HM2013), Lecture Notes in Computer Science (LNCS 7919), pp. 107-117, 2013.

DY 22.4 Wed 15:45 ZEU 160

Semiclassical Spectral Function for Matter Waves in Random Potentials — •Martin-Isbjörn Trappe[1] and Cord Axel Müller[2] — [1]Centre for Quantum Technologies, National University of Singapore — [2]Department of Physics, University of Konstanz, Germany

We derive the first order quantum corrections of the spectral function for matter waves with quadratic dispersion in correlated random potentials using the Wigner function. The spectral density is in particular relevant for the investigation of Anderson localization in laser speckle potentials. The Wigner function approach allows for a systematic semiclassical expansion of the spectral function to arbitrary orders of Planck's constant. We especially consider Gaussian as well as speckle random processes and compare to numerical results. For the case of speckle potentials we present a closed expression for the generating functional.

DY 22.5 Wed 16:00 ZEU 160

Signatures of Symmetry Classes in the Many-Body Transition Amplitude in Fock Space — •Thomas Engl, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

The Bohigas-Giannoni-Schmit (BGS) conjecture states that the energy levels of a single-particle quantum system with classically chaotic counterpart shows the same statistics as that of a Gaussian random matrix satisfying certain symmetries. Semiclassical methods based on the van Vleck-Gutzwiller propagator are able to capture quantum interference effects, and provide a natural route to confirm this conjecture [1]. Therefore, universal effects depending merely on the symmetry class of the described system can be semiclassically understood.

Recently, a semiclassical propagator in Fock space has been derived [2] that accounts for quantum interference in bosonic many body systems. Here we extend this work to interacting fermionic systems and investigate the transition amplitude in Fock space as an indicator of different universality classes. Amongst others, we find an analog of antilocalization for the Gaussian symplectic ensemble corresponding to time reversal invariant spin-1/2 systems.

[1] S. Müller, S. Heusler, A. Altland, P. Braun and F. Haake, New Journal of Physics **11** 103025 (2009)
[2] T. as Engl, J. Dujardin, A. Argüelles, P. Schlagheck, K. Richter and J. D. Urbina, arXiv:1306.3169

DY 22.6 Wed 16:15 ZEU 160

Nonlinear response of a linear chain to weak driving — •Colm Mulhern — Max Planck Institute for the Physics of Complex Systems, Germany

We study the escape of a chain of coupled units over the barrier of a metastable potential. It is demonstrated that a very weak external driving field with suitably chosen frequency suffices to accomplish speedy escape. The latter requires the passage through a transition state the formation of which is triggered by permanent feeding of energy from a phonon background into humps of localised energy and elastic interaction of the arising breather solutions. In fact, cooperativity between the units of the chain entailing coordinated energy transfer is shown to be crucial for enhancing the rate of escape in an extremely effective and low-energy cost way where the effect of entropic localisation and breather coalescence conspire.

15 min break

DY 22.7 Wed 16:45 ZEU 160

From the nonstationarity of the hysteresis memory to a nonstationary response — •Sven Schubert and Günter Radons — TU Chemnitz, 09107 Chemnitz, Germany

A certain memory causes the dependence on the history of an external field and the multistability which are typical features of systems with hysteresis. We consider the number of values N_t stored by hysteresis models, like the Preisach model and the zero-temperature random field Ising model, which are subjected to uncorrelated stationary driving.

The time-dependent probability distribution $P_t(N)$ of the memory length is derived using methods known from record statistics. It is shown that the memory length is on average diverging with time t. Thus, the hysteresis memory caused by uncorrelated stationary noise becomes a nonstationary process, even in the long-time limit.

The nonstationarity of the memory is reflected, for instance, in possible long-time tails in the autocovariance of the stationary response of the Preisach model [1]. Furthermore, the hysteretic response can become a nonstationary process with stationary increments leading on

to $1/f$-noise. We elucidate this mechanism using an example of the symmetric Preisach model and present rigorous results on the power spectral density of the model's response to uncorrelated driving.

[1] G. Radons, Phys. Rev. Lett. **100**, 240602 (2008).

DY 22.8 Wed 17:00 ZEU 160

Density functional theory for elongated polyhedra — •Matthieu Marechal and Klaus Mecke — Friedrich-Alexander-Universität Erlangen-Nürnberg

Due to recent advances in synthesis of nanoparticles and colloids, many-particle system of polyhedra are readily available for experiments. This has spurred a host of many-particle simulation studies on polyhedra. More recently, the lack of theoretical tools to study these system was amended by proposing a density functional theory (DFT) for polyhedra using the frame work of fundamental measure theory.

In this talk, the application of DFT to elongated polyhedra will be discussed. Recent advancements in the DFT of long rods allow us to consider nematic and smectic liquid crystals in addition to the isotropic phase. We will first consider these phases for triangular prisms that are elongated along their rotation axis. We validate the DFT approach by comparing to Monte Carlo computer simulations and we calculate the liquid crystal phase diagram.

Colloidal prisms with arbitrarily shaped bases have been synthesized using nanolithography; our DFT approach allows to explore the enormous ensuing shape parameter space. We focus on smectic phases and determine which shapes show a global tilt between the particle direction and the layer normal ('smectic C') or a splitting of the layer into two layers (bilayer smectic). We hope our results motivate further experiments on colloidal smectics.

DY 22.9 Wed 17:15 ZEU 160

2D Melting in General: Solid/hexatic/liquid Phase Transitions in Soft Spheres using Event-Chain Monte Carlo — •Sebastian C Kapfer, Manon Michel, and Werner Krauth — LPS, Ecole normale supérieure, Paris, France

The melting transition of two-dimensional solids has been the subject of continued research for more than fifty years, with the prevalent scenarios being the KTHNY theory of defect unbindung and a conventional first-order liquid/solid transition. For hard disks, a rather unexpected hybrid transition has recently been found with both a first-order transition and an intermediate hexatic phase [1], while magnetic colloid experiments support the KTHNY scenario [2]. To resolve this discrepancy, we here address the melting problem for soft interaction potentials, in particular the nature of the liquid/hexatic and hexatic/solid transitions, and the defects driving melting. Simulations were effected by a new rejection-free irreversible Monte Carlo algorithm generalizing event-chain Monte Carlo to soft arbitrary pair potentials. In addition to fast equilibration, this algorithm allows to deduce pressure in the NVT ensemble without any additional computations [3].

[1] E. P. Bernard, W. Krauth, Phys. Rev. Lett. 107, 155704 (2011). [2] P. Keim et al. Phys. Rev. Lett. 92, 215504 (2004). [3] M. Michel et al., preprint at arXiv:1309.7748.

DY 22.10 Wed 17:30 ZEU 160

Ising Kagome Paramagnet is a Mean-Field system — •Taras Yavors'kii — AMRC, Department of Mathematics and Physics, Coventry University, CV1 5FB, England

Antiferromagnetic nearest-neighbor Ising model on a geometrically frustrated two-dimensional kagome lattice does not order down to $T = 0$ [1]. Using Monte Carlo simulations on graphics processing units (GPUs) as a tool, I show that statistical physics properties of the model, including pair correlation function and specific heat, are well described by the variational single-particle mean-field theory [2] (MFT) ansatz at *all* $T \geq 0$, provided the MFT temperature scale Θ, where $\Theta_c < \Theta < \infty$, is mapped onto the physical temperature scale $0 \leq T < \infty$ by considering Θ as a suitable function of T. The model is thus completely "transparent" to the paramagnetic MFT treatment deep below the MFT critical temperature $\Theta_c > 0$, making MFT a simple and powerful tool for the study of perturbations at low T.

[1] K. Kanô and S. Naya, *Prog. Theor. Phys.* **10** 158 (1953)

[2] P. M. Chaikin and T. C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, Cambridge, UK, 1995)

DY 22.11 Wed 17:45 ZEU 160

A Maxwell's demon action on a tape with energy exchange — •Johannes Hoppenau — Carl-von-Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Currently, in statistical physics, models that incorporate information processing are of lively interest. Several of these models consider an information carrying tape. Typically, it is assumed that no energy is needed to store information on this tape. We investigate how things change, if this assumption is relaxed. Therefore, we propose a model of a tape, where the information is encoded in a two-level systems, via its energystates. In this model energy is needed to write information. Our focus is on the efficiency of devices that are coupled to such a tape. We derive an upper bound for the efficiency, which is more restrictive than the Carnot bound. This bound holds whether or not the model contain feedback.

DY 22.12 Wed 18:00 ZEU 160

Approximative counting of Manifold Triangulations — •Benedikt Krüger and Klaus Mecke — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Each topological manifold in 2d and 3d permits a finite number of non-equivalent discretisations into combinatorial manifolds or triangulations with given number of vertices or maximal simplices. This number of distinct triangulations is important for questions arising in topology, geometry and physics. e.g. in quantum gravity [1].

Until now the best method for the counting of combinatorial manifolds was the isomorphism free enumeration of all possible triangulations which succeeded for vertex numbers below about 15 [2]. We use Monte-Carlo algorithms for estimating the number of triangulations of two- and three-dimensional manifolds and show that we are able to increase the known regime of triangulation counts by one magnitude. We give numerical evidence that the number of surface triangulations scales exponentially with the vertex number and that the rate of growth depends linearly on the genus of the surface.

[1] J. Ambjørn, J. Jurkiewicz, and R. Loll, Phys. Rev. D 72, 064014 (2005)

[2] T. Sulanke and F. H. Lutz, Eur. J. Comb. 30, 1965 (2009)

DY 23: Quantum Chaos

Time: Wednesday 15:00–18:45 Location: ZEU 146

DY 23.1 Wed 15:00 ZEU 146

Spectral properties of microwave graphs with absorption — Markus Allgeier[1], Stefan Gehler[1], Sonja Barkhofen[1,3], Ulrich Kuhl[1,2], and •Hans-Jürgen Stöckmann[1] — [1]Fachbereich Physik, Universität Marburg — [2]Université de Nice Sophia-Antipolis, Nice, France — [3]Fachbereich Physik, Universität Paderborn

The influence of absorption on the spectra of microwave graphs has been studied experimentally. The microwave networks were made up of coaxial cables and T junctions. First, absorption was introduced attaching a 50 Ohm load to an additional vertex for graphs with and without time-reversal symmetry. The resulting level spacings distributions were compared with a generalization of the Wigner surmise in the presence of open channels proposed recently by Poli et al. [1]. A good agreement was found using an effective coupling parameter. Secondly, absorption was introduced along one individual bond via a variable microwave attenuator, and the influence of absorption on the length spectrum was studied. The peak heights in the length spectra corresponding to orbits avoiding the absorber were found to be independent of the attenuation, whereas the heights of peaks belonging to orbits passing the absorber once or twice showed the expected decrease with increasing attenuation.

[1] Poli et al., Phys. Rev. Lett. 108, 174101 (2012)

DY 23.2 Wed 15:15 ZEU 146

Experimental realization of superconducting quantum graphs — Barbara Dietz-Pilatus, Maksym Miski-Oglu, •Tetyana Skipa, and Achim Richter — Technische Universität Darmstadt, Institut für Kernphysik, Schlossgartenstraße 9, 64289 Darmstadt

We report on the design of superconducting quantum graphs, which will be realized with networks of two-dimensional microwave waveguides. We compare numerical results for the eigenvalue spectrum of microwave networks with that of the corresponding quantum graphs. Furthermore, the complete scattering matrix (S-matrix) of the microwave network was calculated and its properties are compared with theoretical predictions for the occurrence of topological resonances in open quantum graphs [1] and higher order correlation functions of the S-matrix [2]. The numerical calculations were performed with CST MW Studio. The scattering matrix is planned to be measured experimentally with superconducting microwave networks at liquid helium temperature in the frequency range from 14 to 40 GHz. This work was supported by the DFG within the Sonderforschungsbereich 634.

[1] S. Gnutzmann, H. Schanz and U. Smilansky, Phys. Rev. Lett. 110, 094101 (2013) [2] Z. Pluhar, H. A. Weidenmueller, Phys. Rev. Lett. 110, 034101 (2013)

DY 23.3 Wed 15:30 ZEU 146

Quantum graphs whose spectra mimic the zeros of the Riemann zeta function — •Jack Kuipers, Quirin Hummel, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

One of the most famous problems in mathematics is the Riemann hypothesis: that the non-trivial zeros of the Riemann zeta function lie on a line in the complex plane. One way to prove the hypothesis would be to identify the zeros as eigenvalues of a Hermitian operator, many of whose properties can be derived through the analogy to quantum chaos. Using this, we construct a set of quantum graphs that have the same oscillating part of the density of states as the Riemann zeros, offering an explanation of the overall minus sign. The smooth part is completely different, and hence also the spectrum, but the graphs pick out the low-lying zeros.

arXiv:1307.6055

DY 23.4 Wed 15:45 ZEU 146

Time multiplexed photonic quantum walks — Andreas Schreiber[1,2], Fabian Katzschmann[1], •Sonja Barkhofen[1], Aurél Gábris[3], Peter Rohde[1], Kaisa Laiho[1,2], Martin Stefanák[3], Václav Potocek[3], Craig Hamilton[3], Igor Jex[3], and Christine Silberhorn[1] — [1]Applied Physics, University of Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Max-Planck-Institute for the Science of Light, Günther-Scharowsky-Str. 1 / Bau 24, 91058 Erlangen, Germany — [3]Department of Physics, Faculty of NuclearSciences and Physical Engineering, Czech Technical University in Prague, Brehová 7, 115 19 Praha, Czech Republic

Linear optical networks which comprise a large number of optical modes have been investigated intensively in various theoretical proposals. Most recently their relevance for studies of photonic quantum walk systems has attracted attention, because they can be considered as a standard model to describe the dynamics of quantum particles in a discretized environment and serve as a simulator for other quantum systems, which are not as readily accessible. A key element for a versatile simulator is the ability to dynamically control the quantum-coin, which is the main entity responsible for the evolution of the quantum walk. The utilization of the polarization state as coin state allows for easy manipulation by introducing controlled phase shifts through an electro optic modulator to selectively modify the coin state. This enables us to tune interaction strengths and patterns to simulate different kinds of particles or environments and thus enhancing the abilities of photonic experiments.

DY 23.5 Wed 16:00 ZEU 146

Asymmetric backscattering in waveguide-coupled microdisk resonators — •Johannes Kramer and Jan Wiersig — Otto-von-Guericke-Universität Magdeburg, 39016 Magdeburg

Recently, it has been discovered that the coherent backscattering of counter-propagating waves in deformed or perturbed microdisk cavities can be asymmetric provided that the cavity does not possess a mirror-reflection symmetry [1,2]. This leads to the appearance of nonorthogonal pairs of copropagating optical modes with a preferred sense of rotation. In the extreme case the pair of modes coalesce at a so-called exceptional point. We present finite-difference time-domain (FDTD) simulations which indicate that the asymmetric backscattering can be unambiguously identified in transmission and reflection experiments on waveguide-coupled microdisks.

[1] J. Wiersig, A. Eberspächer, J.-B. Shim, J.-W. Ryu, S. Shinohara, M. Hentschel, and H. Schomerus, Phys. Rev. A 84, 023845 (2011)
[2] J. Wiersig, Phys. Rev. A 84, 063828 (2011)

DY 23.6 Wed 16:15 ZEU 146

Manifestation of periodic orbits in triangular microlasers — •Stefan Bittner[1], Clément Lafargue[1], Christian Ulysse[2], Alain Grigis[3], Joseph Zyss[1], and Mélanie Lebental[1] — [1]Quantum and Molecular Photonics Laboratory, ENS Cachan — [2]Laboratory for Photonics and Nanostructures, Marcoussis — [3]Laboratoire Analyse, Géométrie et Applications, University Paris 13

One of the main interests in open dielectric resonators is to understand the correspondence between their wave dynamics and the classical ray dynamics. We present experiments with flat organic microlasers of triangular shape. The aim of the experiments was to understand the relation between the lasing properties of the microlasers and the periodic orbits (POs) in the corresponding triangular billiards. Triangles are of special interest since they are the most simple polygons and because the number and types of POs in general triangular billiards remain unknown. The spectra and far-field distributions of the microlasers were measured and photographs of the lasing cavities themselves were taken. These data allowed to identify the underlying POs. Several types of triangles with different kinds of classical dynamics and POs were studied. In some cases all lasing modes were based on a single family of POs whereas in other cases a competition between modes based on different types of POs was observed. Furthermore, some lasing modes seemed to be based on diffractive POs, i.e., orbits that impinge directly on a diffractive corner. Such modes could be used as a tool to further investigate the diffraction at dielectric corners.

DY 23.7 Wed 16:30 ZEU 146

Goos-Hänchen shift and Fresnel filtering at curved interfaces - Analytic and numeric results — •Pia Adam, Jakob Kreismann, and Martina Hentschel — Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany

Describing confined light bundles by rays obeying the laws of geometrical optics is a powerful tool even in the regime where, strictly speaking, full wave dynamics should be applied. When considering structures at length scales of a few wavelengths, however, semiclassical effects have to be taken into account. These deviations from the laws of geometrical optics are the Goos-Hänchen shift which is long known

for planar interfaces, and the Fresnel filtering effect. In this work we derive analytical expressions to describe the Goos-Hänchen shift and Fresnel filtering at curved interfaces in the regime of total reflection as well as for partial reflection. These analytical results are supported by numerical simulations.

15 min break

DY 23.8 Wed 17:00 ZEU 146

Resonance chains in the open 3-disk system — •Tobias Weich[2], Sonja Barkhofen[1], Ulrich Kuhl[3], Charles Poli[4], and Henning Schomerus[4] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5,35032 Marburg, Germany — [2]Fachbereich Mathematik, Philipps-Universität Marburg, Hans-Meerwein-Straße,35032 Marburg, Germany — [3]Laboratoire de Physique de la Matière Condensée, CNRS UMR 7336, Université de NiceSophia-Antipolis, F-06108 Nice, France — [4]Department of Physics, Lancaster University, Lancaster LA1 4YB, UK

In ballistic open quantum systems one often observes that the resonances in the complex-energy plane form a clear chain structure. Taking the open 3-disk system as a paradigmatic model system, we investigate how this chain structure is reflected in the scattering states and how it is connected to the underlying classical dynamics. Furthermore we present a simple open quantum graph model consisting of two edges that shows surprisingly similar behaviour in its resonance structure and scattering states.

DY 23.9 Wed 17:15 ZEU 146

Multifractals in Quantum Chaos — •Moritz Schönwetter and Eduardo G. Altmann — MPIPKS, Dresden

Fractal properties of open chaotic systems are known to play an important role in their corresponding quantum systems. Well studied examples are the localisation of long lived states on fractal structures in the classical phase space and the fractal Weyl law connecting the asymptotic resonance density with the fractal dimension D_0 of the classical invariant set. In numerous physically relevant cases the opening is not complete but results from partial absorption and partial reflection (e.g., of the intensity of optical rays), in which case the classical system is no longer characterised by D_0 but by the full multi-fractal spectrum of Rényi dimensions D_q. Here we study the influence of partial reflection and multi-fractality of the underlying classical system on spectral properties of the quantum mechanical counterpart.

DY 23.10 Wed 17:30 ZEU 146

Hierarchical Resonance States and Fractal Weyl Laws — •Martin Körber[1], Matthias Michler[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]Technische Universität Dresden, Institut für Theoretische Physik, 01062 Dresden, Germany — [2]MPI für Physik komplexer Systeme, 01187 Dresden, Germany

The chaotic dynamics of generic Hamiltonian systems is governed by partial barriers. They also strongly influence the system's quantum-mechanical properties. In closed systems, the localization of eigenstates around a partial barrier universally depends on the ratio of the flux across the partial barrier and the effective size of Planck's cell, only [1]. In open systems, however, we observe that partial barriers imply localization of resonance states apart from this criterion. This gives rise to hierarchical fractal Weyl laws in generic systems [2]. We present an argument for the existence of these localized resonance states and study their parameter dependence. We design a model system that allows us to distinguish between the universal influence of the opening and the subtle contribution from the chaotic saddle.

[1] Phys. Rev. Lett. **109**, 234101 (2012)
[2] Phys. Rev. Lett. **111**, 114102 (2013)

DY 23.11 Wed 17:45 ZEU 146

The Weyl expansion for systems of identical particles - Spatial Friedel oscillations for excited many-body states — •Quirin Hummel, Juan Diego Urbina, Markus Biberger, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

For single-particle billiard systems, the smooth part of the density of states (DOS) in a semiclassical approximation is known as the Weyl expansion. In [1] we study a corresponding expansion for the smooth part of the many-body DOS in fermionic and bosonic systems including physical boundary effects. Here, we exploit this framework to give formal and explicit expressions for the smooth part of the local density of states (LDOS) in such systems. Comparing the many-body LDOS with the average behaviour of the spatial density of a system of non-interacting fermions near the ground state, known as Friedel oscillations, we show that our expressions can be understood as an extension of the latter to excited many-body energies.

[1] arXiv 1210.5748

DY 23.12 Wed 18:00 ZEU 146

Resonance Assisted Tunneling in Mixed Systems using Integrable Approximations — •Clemens Löbner[1,2], Julius Kullig[1], Normann Mertig[1,2], Steffen Löck[1,3], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]Technische Universität Dresden, Institut für Theoretische Physik, 01062 Dresden — [2]MPI für Physik komplexer Systeme, 01187 Dresden — [3]Technische Universität Dresden, Oncoray - National Center for Radiation Research in Oncology, 01307 Dresden

Generic Hamiltonian systems have a mixed phase space in which regions of regular motion are embedded in regions of chaotic motion. Quantum mechanically these regions are connected by regular-to-chaotic tunneling. In the presence of nonlinear resonances, this effect is strongly enhanced and is therefore called resonance-assisted tunneling.

We present a theoretical description of resonance-assisted tunneling in mixed systems using an integrable approximation of the regular region. We introduce a new method [1] based on canonical transformations to construct the integrable approximation and extend this method to systems with resonances. The resulting approximation is used for the prediction of regular-to-chaotic tunneling rates. We show results for the generic standard map.

[1] C. Löbner, S. Löck, A. Bäcker, and R. Ketzmerick: Phys. Rev. E 88, 062901 (2013)

DY 23.13 Wed 18:15 ZEU 146

Semiclassical theory of bosonic many-body scattering: a non-perturbative Green's function approach — •Josef Michl, Thomas Engl, Markus Biberger, Juan-Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

Semiclassical techniques have so far been applied mainly to single-particle systems. For these systems they provide a powerful toolbox to study interference effects and allow for analytical calculations even in the presence of classical chaos.
Previously, we have succeeded in constructing a semiclassical approximation of the propagator in bosonic Fock state representation which is based on real actions and hence shows interference in Fock space explicitly[1]. This opens the possibility to define semiclassical many-body Green's functions, the natural objects required to study stationary many-body scattering. The main advantage of such an approach is that it provides a non-perturbative method to address directly the full many-body Green's function, contrary to standard methods based on Dyson expansions. However, this program requires a proper theory of many-body scattering, beyond the usual picture based on single-particle observables like the current. We present an overview of the conceptual and technical basis of many-body stationary scattering, and show how the many-body semiclassical Green's function can be used in this context.

[1] Thomas Engl *et al.*, arXiv:1306.3169.

DY 23.14 Wed 18:30 ZEU 146

Quantum-classical correspondence and critical phenomena in anisotropic Kepler problem — •Kazuhiro Kubo — Max-Planck-Institut für Physik Komplexer Systeme, Dresden, Germany

Recently the importance of entanglement analysis in the Anderson localization is well recognized with respect to the multifractality of a wave function near the criticality. From a random matrix model for the critical statistics, García-García and Verbaarschot conjectured in 2003 that the Anderson localization closely relates to the critical phenomena in the quantum chaos. The crucial test can be done by investigating the relation between the wave function multifractality and the compressibility of energy eigenvalues. As a suitable model we choose the anisotropic Kepler problem (AKP) — the hydrogen atom with electron-mass anisotropy parameter. We have recently performed an extensive numerical calculation for the AKP quantum states using two independent basis sets (sturmian and harmonic-wave function basses). We hope we can present a preliminary account on this issue.

DY 24: Networks - Statistics and Dynamics (joint session DY/ BP/ SOE)

Time: Wednesday 15:00–18:45 Location: ZEU 118

DY 24.1 Wed 15:00 ZEU 118

Chimera states: spontaneous symmetry-breaking in dynamical networks — •Eckehard Schöll — Institut für Theoretische Physik, TU Berlin, Hardenbergstr 36, 10623 Berlin, Germany

Systems of nonlocally coupled identical oscillators can exhibit symmetry-breaking in the form of complex spatiotemporal patterns, called chimera states, which consist of coexisting domains of spatially coherent (synchronized) and incoherent (desynchronized) dynamics. We describe the scenario leading from complete coherence to complete incoherence via chimera states [1,2], and present a general analytical calculation of the critical coupling strength at the onset of the chimera states.

[1] I. Omelchenko, Y. Maistrenko, P. Hövel, and E. Schöll: Loss of coherence in dynamical networks: spatial chaos and chimera states, Phys. Rev. Lett. 106, 234102 (2011).

[2] A. Hagerstrom, T.E. Murphy, R. Roy, P. Hövel, I. Omelchenko, and E. Schöll: Experimental observation of chimeras in coupled-map lattices. Nature Physics 8, 658 (2012)

Work in collaboration with A. Hagerstrom, P. Hövel, K. Krischer, Y. Maistrenko, T.E. Murphy, I. Omelchenko, O.E. Omel'chenko, R. Roy, A. Zakharova.

DY 24.2 Wed 15:15 ZEU 118

Pattern-matching via a network of phase oscillators of different frequency: A novel Architecture — •Daniel Heger and Katharina Krischer — Technische Universität München, Physikdepartment

Oscillatory networks can in principle be used for pattern recognition. Nevertheless, current architectures either lack scalability towards large numbers of oscillators or need the external input of complex time-dependent coupling functions. In our talk, we will present a novel architecture for pattern matching with oscillatory neural networks. A system of oscillators of different frequencies and coupling functions is used whose dynamics average to the dynamics of an all-to-all coupled oscillator network. In contrast to previous approaches, the necessary coupling functions are automatically generated inside the network and the output pattern can easily be read out binary. By additionally choosing a new type of coupling function, the matching mechanism is stable even for high coupling strengths and the degenerate attractive limit set containing the memorized patterns transforms to a system of seperated attractors for each memorized pattern. Although the system's dynamics do not average to the dynamics of simple coupled Kuramoto oscillators, the appealing mathematical structure permits determination of the stability of all fixed points using nonlinear stability analysis and a dynamic equation solely in pattern space can be derived.

DY 24.3 Wed 15:30 ZEU 118

Data acquistion by vectorization of high resolution images of vascular networks — •Jana Lasser — Max-Planck-Institut für Dynamik und Selbstorganisation

Leaf vein networks form highly complex, reticulate, hierarchically organized webs that are believed to be the result of a process of gradual optimization over the course of evolutionary history. These networks form planar graphs dominated by cycles, but to this day the topological properties of such reticulate networks have not been adequately described. We analyze the hierarchical organization of the loops in transport networks from roughly 100 cleared leaf images that are converted into a weighted graph representation using custom tailor-made image analysis tools. We employ tools from statistics and topology, in particular an algorithmic way of assigning a topological tree graph to the leaf's loop graph which represents its hierarchical organization, thus allowing us to make use of specialized tree metrics to unravel the distinguishing characteristics between different network realisations. Our algorithmic tools allow us to quantitatively describe subtle differences between venation phenotypes, and compare reticulate network data with the predictions of optimisation models.

DY 24.4 Wed 15:45 ZEU 118

Structure and Topology of Optimal Transport Networks in Plant Leaves — •Henrik Ronellenfitsch and Eleni Katifori — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Efficient photosynthesis in plants crucially depends on the ability to transport water from the soil into the leaves, where it can evaporate. To this effect, plants are equipped with a network of pipe-like cells, the xylem, facilitating efficient delivery of water to all parts of the organism. In the leaf, these networks form highly complex, highly reticulate, hierarchically organized webs that are believed to be the result of a process of gradual optimization over the course of evolutionary history. Based on the assumption of functional optimization over the course of evolution, we construct models for optimal transport networks adapted to different kinds of damage (modelling herbivory, diseases, etc...) and fluctuating load (modelling the fact that the stomata, small orifices responsible for the exchange of gasses, open in patches at a time). We numerically solve the resulting optimization problem and analyze the solutions with special regard to structure and hierarchical organization of loops which arise in response to damage and fluctuations.

DY 24.5 Wed 16:00 ZEU 118

The topology of adaptively controlled networks — •Judith Lehnert[1], Philipp Hövel[1,2], Alexander Fradkov[3,4], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Bernstein Center for Computational Neuroscience, HU Berlin, Philippstr. 13, 10115 Berlin, Germany — [3]SPb State University, Universitetskii pr.28, St. Petersburg, 198504 Russia — [4]Institute for Problems of Mechanical Engineering, Russian Academy of Sciences, Bolshoy Ave, 61, V. O., St. Petersburg, 199178 Russia

Adaptive networks are characterized by a complicated interplay between the dynamics of the nodes and a changing topology: The topology evolves according to the state of the system, while at the same time the dynamics on the network and thus its state is influenced by that topology. Here, we present an algorithm for a changing topology that allows us to control the dynamics on the network. In particular, we control zero-lag and cluster synchronization in delay-coupled networks of Stuart-Landau oscillators.

The emerging topology of the network is modulated by the delay. If the delay time is a multiple of the system's eigenperiod, the coupling within a cluster and to neighboring clusters is on average positive (excitatory), while the coupling to clusters with a phase lag close to π is negative (inhibitory). For delay times equal to odd multiples of half of the eigenperiod, we find the opposite: Nodes within one cluster and of neighboring clusters are coupled by inhibitory links, while the coupling to clusters distant in phase state is excitatory.

DY 24.6 Wed 16:15 ZEU 118

Hierarchical block structures and high-resolution model selection in large networks — •Tiago P. Peixoto — Universität Bremen, Germany

Many social, technological, and biological networks are composed of modules, which represent groups of nodes which have a similar role in the functioning of the network. The problem of detecting and characterizing these modules is a central one in the broad field of complex systems. However most existing methods used to obtain the modular structure of networks suffer from serious problems, such as the resolution limit on the size of communities. This phenomenon occurs for the very popular approach of modularity optimization, but also for more principled ones based on statistical inference and model selection. Here I construct a nested generative model which, through a complete description of the entire network hierarchy at multiple scales, is capable of avoiding this limitation, and enables the detection of modular structure at levels far beyond those possible by current approaches. Even with this increased resolution, the method is based on the principle of parsimony, and is capable of separating signal from noise. Furthermore, it fully generalizes other approaches in that it is not restricted to purely assortative mixing patterns, directed or undirected graphs, and ad hoc hierarchical structures such as binary trees..

References: [1] Tiago P. Peixoto, Phys. Rev. Lett. 110 14 148701 (2013); [2] Tiago P. Peixoto, arXiv: 1310.4377; [3] Tiago P. Peixoto, arXiv: 1310.4378

DY 24.7 Wed 16:30 ZEU 118

Temporal networks: Laplacian spectra and synchroniza-

tion — •Konstantin Klemm[1,2], Naoki Masuda[3], and Victor M. Eguiluz[4] — [1]Bioinformatics, Institute of Computer Science, Leipzig University, Germany — [2]Bioinformatics and Computational Biology, University of Vienna, Austria — [3]Department of Mathematical Informatics, The University of Tokyo, Japan — [4]Instituto de Fisica Interdisciplinar y Sistemas Complejos, Palma de Mallorca, Spain

Interactions among units in complex systems occur in a specific sequential order thus affecting the flow of information, the propagation of diseases, and general dynamical processes. We investigate the Laplacian spectrum of temporal networks and compare it with that of the corresponding aggregate network. First, we show that the spectrum of the ensemble average of a temporal network has identical eigenmodes but smaller eigenvalues than the aggregate networks. In large networks without edge condensation, the expected temporal dynamics is a time-rescaled version of the aggregate dynamics. Even for single sequential realizations, diffusive dynamics is slower in temporal networks [1]. These discrepancies are due to the noncommutability of interactions. The final part of the presentation uses the calculated spectra to predict the stability of non linear-systems with diffusive temporal couplings.

[1] N. Masuda, K. Klemm, V. M. Eguiluz, Phys. Rev. Lett. 111, 188701 (2013).

15 min break

DY 24.8 Wed 17:00 ZEU 118

Phase Transitions in Cooperative Coinfections: Simulation Results for Networks and Lattices — •Weiran Cai[1], Li Chen[2,3], Fakhteh Ghanbarnejad[2], and Peter Grassberger[4] — [1]Faculty of Electrical and Computer Engineering, Technische Universität Dresden, Germany — [2]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [3]Robert Koch-Institut P4 - Epidemiologische Modellierung von Infektionskrankheiten, Berlin, Germany — [4]JSC, FZ Jülich, D-52425 Jülich, Germany

In this talk, we study the spreading of a cooperative coinfection on different networks topologies. Previous work has shown that in a mean field approximation, the cooperativity of two diseases in the SIR framework can lead to first-order transitions, where the relative size of the infected cluster changes discontinuously with respect to control parameters. However, due to the mean field approximation, such discontinuous transitions could occur only when the initial density of infected sites is finite. Here we show that the same is true on trees, but not on other networks. On Erdős-Renyi(ER) networks, on networks with long range contacts, and lattices with dimension = 3 we find first order transitions initiated even by a single sick site, while no first order transitions are observed on 2-dimensional lattices, if the contacts are short range. The importance of loops for the presence/absence of discontinuous transitions is discussed.

DY 24.9 Wed 17:15 ZEU 118

Stability of Boolean and continuous dynamics — •Fakhteh Ghanbarnejad[1] and Konsatntin Klemm[2,3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Bioinformatics, Institute for Computer Science, University of Leipzig, Germany — [3]Institute for Theoretical Chemistry, University of Vienna, Austria

Regulatory dynamics in biology is often described by continuous rate equations for continuously varying chemical concentrations. Binary discretization of state space and time leads to Boolean dynamics. In the latter, the dynamics has been called unstable if flip perturbations lead to damage spreading. Here, we find that this stability classification strongly differs from the stability properties of the original continuous dynamics under small perturbations of the state vector. In particular, random networks of nodes with large sensitivity yield stable dynamics under small perturbations. (Phys. Rev. Lett. 107, 188701 (2011))

DY 24.10 Wed 17:30 ZEU 118

Physiological networks studied with time-delay stability analysis — •Jan W. Kantelhardt[1], Amir Bashan[2], Ronny P. Bartsch[3], Shlomo Havlin[2], and Plamen C. Ivanov[3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Department of Physics, Bar-Ilan University, Israel — [3]Harvard Medical School, Boston, USA

The human organism is an integrated network where complex physiological systems, each with its own regulatory mechanisms, continuously interact, and where failure of one system can trigger a breakdown of the entire network. Identifying and quantifying dynamical networks of diverse systems with different types of interactions is a challenge. We have developed time-delay stability analysis as a framework to probe interactions among diverse systems and identified a physiological network from recorded time series data. Each physiological state is characterized by a specific network structure, demonstrating a robust interplay between network topology and function. Across physiological states, the network undergoes topological transitions associated with fast reorganization of physiological interactions on time scales of a few minutes, indicating high network flexibility in response to perturbations.

DY 24.11 Wed 17:45 ZEU 118

Large networks have small Problems — •Helge Aufderheide[1] and Thilo Gross[2] — [1]Max-Planck Institut für Physik komlpexer Systeme — [2]University of Bristol, MV School of Engineering Mathematics

On several levels, humans depend on the functioning of complex networks, such as food webs and technical infrastructure networks. However, recent work shows that trying to stabilize a network can lead to large-scale failures. This suggests that it is important to assess not only the risk of a failure, but also its scale. Here we show that instabilities which naturally occur in large networks are typically localized, such that they affect only a relatively small part of the network directly, whereas attempts to stabilize the network can lead to a delocalization, such that instabilities are less likely but will affect a larger number of nodes when they occur. These results may explain how many natural networks can stabilize themselves by sacrificing the parts in which instabilities occur, whereas cases of delocalized systemic failure are known to occur in artificial technical or organizational networks.

DY 24.12 Wed 18:00 ZEU 118

Outbreaks of coinfections: the critical role of cooperativity — •Fakhteh Ghanbarnejad[1], Li Chen[1], Weiran Cai[2], and Peter Grassberger[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Faculty of Electrical and Computer Engineering, TU Dresden, Germany — [3]JSC, FZ Jülich, D-52425 Jülich, Germany

Modeling epidemic dynamics plays an important role in studying how diseases spread, predicting their future course, and designing strategies to control them. In this talk, we introduce a model of SIR (susceptible-infected-removed) type which explicitly incorporates the effect of *cooperative coinfection*. More precisely, each individual can get infected by two different diseases, and an individual already infected with one disease has an increased probability to get infected by the other. Depending on the amount of this increase, we prove different threshold scenarios. Apart from the standard continuous phase transition for single disease outbreaks, we observe continuous transitions where both diseases must coexist, but also discontinuous transitions are observed, where a finite fraction of the population is already affected by both diseases at the threshold. All our results are obtained in a mean field model using rate equations, but we argue that they should hold also in more general frameworks. (arXiv:1307.2404)

DY 24.13 Wed 18:15 ZEU 118

Onset of self-sustained activity in a simple model of excitable dynamics on graphs — •Christoph Fretter[1,2], Annick Lesne[3], Claus C. Hilgetag[1,4], and Marc-Thorsten Hütt[2] — [1]Department of Computational Neuroscience, Universitätsklinikum Hamburg-Eppendorf, Hamburg, Germany — [2]School of Engineering and Science, Jacobs University Bremen, Germany — [3]LPTMC UMR 7600, Université Pierre et Marie Curie-Paris 6, 4 place Jussieu, F-75252 Paris, France — [4]Department of Health Sciences, Boston Uniersity, Boston, USA

Models of simple excitable dynamics on graphs are an efficient framework for studying the interplay between network topology and dynamics. This subject is a topic of practical relevance to diverse fields, ranging from neuroscience to engineering. Using a discrete excitable node model, we analyse how a single excitation propagates through a random network as a function of the excitation threshold,that is, the percentage of excitations in the neighborhood required for an excitation of a node. Using numerical simulations and analytical considerations, we can understand the onset of sustained activity as an interplay between topological cycle statistics and path statistics. Our findings are interpreted in the context of the theory of network reverberations in neural systems, which is a question of long-standing interest in computational neuroscience.

DY 24.14 Wed 18:30 ZEU 118

Laplacian Spectrum of 2d Lattice Triangulations — •Ella Schmidt, Benedikt Krüger, and Klaus Mecke — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Triangulations are an important tool in physics for describing curved geometries. Unimodular triangulations on 2d lattices can also be considered as connected, simple, plane graphs, which allows the appliance of methods from spectral graph theory on triangulations.

We calculate the distribution and averages of eigenvalues of the Laplacian matrix for random and highly ordered unimodular triangulations. Introducing a curvature energy of triangulations we measure microcanonical and canonical averages of the eigenvalues using Monte-Carlo-Simulations. We examine the probability distributions of the spectra of the ensembles of triangulations, the dependence of the eigenvalues on energy and temperature as well as the scaling with the lattice size and compare with random graph models.

In the microcanonical ensemble we find in agreement with our analytical predicitions a linear dependence of the algebraic connectivity and the spectral radius on the energy, in the canonical ensemble we encounter quasi-critical behaviour.

DY 25: Symposium SYEE: Energy Meets Economy: Dynamics and Statistics of Future Energy Systems (joint session SOE/ DY)

Time: Wednesday 15:00–17:45 Location: HSZ 02

Invited Talk DY 25.1 Wed 15:00 HSZ 02

Smart Grids - From incentives to coupled markets — •Rudolf Sollacher — Siemens AG, Corporate Technology, Munich, Germany

Future energy systems must meet the challenges introduced by an increasing portion of distributed renewable power generation. This talk describes the main challenges and presents current and future solutions. A special focus will be on market based approaches.

Invited Talk DY 25.2 Wed 15:30 HSZ 02

Energy and the economy — •Reiner Kümmel — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg

Energy conversion and entropy production determine the growth of wealth in industrialized economies. Novel econometric analyses have revealed energy as a production factor whose output elasticity, which measures its economic weight, is much larger than its share in total factor cost, while for labor just the opposite is true. Although this result is at variance with neoclassical economic theory, it is compatible with the standard maximization of profit or time-integrated utility, if one takes technological constraints on capital, labor, and energy into account.

Invited Talk DY 25.3 Wed 16:00 HSZ 02

Planetary constraints to energy supply and the economy — •Oliver Richters — Universität Oldenburg, Institut für Chemie und Biologie des Meeres, Theoretische Physik / Komplexe Systeme — Vereinigung für Ökologische Ökonomie

The "great transformation" towards a future proof economy depends on the provision of a sustainable energy supply. Different planetary boundaries restrict the phase space of possible technical and sociatal solutions. Solar energy or nuclear fusion appear to be the solution for the radical reduction of greenhouse gas emissions, disregarding that other problem areas persist: First, the excessive installation of photovoltaics enters into competition with other kind of landuse and therefore may lead to land system change and accelerate biodiversity loss. Second, the low entropy of solar radiation is the basis for life on earth and its harvesting for human activity reduces the energy available for biological and meteorological processes. Jointly, though renewables can't run out of stock, the energy throughput is constrained by the speed of regeneration. Third, even nuclear fusion or other sun-independent energy supply cause global warming simply by thermal pollution, as every human activity finally ends up as heat. On the whole, this poses relevant limitations to world energy consumption and possible future energy systems. The realisation of a sustainable energy supply will stop the excessive growth of energy throughput, putting relevant constraints to economic growth, so that it will probably come to an end. An insight is given into the significance this development has for finance, economics, social security and the people on earth.

- 15 minutes break -

Invited Talk DY 25.4 Wed 16:45 HSZ 02

Identifying critical infrastructures in complex supply networks — •Dirk Witthaut — Institut für Energie- und Klimaforschung, Forschungszentrum Jülich — Institut für theoretische Physik, Universität zu Köln — Max-Planck-Institut für Dynamik und Selbstorganisation

Transmission line failures can induce large-scale outages in power grids and other complex supply networks, causing potentially huge economic losses. Yet, how to determine which lines are particularly sensitive to inducing larger-scale outages is currently not well understood. In this talk I will discuss how the topological redundancy of a transmission line limits dynamical network robustness and allows to reliably identify critical infrastructures. I derive criteria to predict the dynamic stability of power grids based on the networks topology and the static loads prior to line failure. As both criteria are available before any outage from the state of normal operation, they may support network planning and real-time monitoring of grid operation.

Invited Talk DY 25.5 Wed 17:15 HSZ 02

Short time fluctuations of renewable energies — •Joachim Peinke, M. Reza Rahimi Tabar, Patrick Milan, and Matthias Wächter — Institut für Physik und ForWind, Universität Oldenburg, Germany

Wind and solar energy, the main renewable energies on which the modern sustainable electrical power supply will be based, are characterized by a high volatility. News report frequently on a new challenge for the energy management to handle these new sources. For a better understanding of their impact on the electrical power system it is essential to know in more details the nature of the power fluctuations of wind and solar energy.

In our contribution we present results from an analysis of wind and solar power. We show that the turbulent features of the weather can be seen in the power output of such systems. We will mainly focus on the characterization and modeling of these power systems with advanced stochastic tools. Concerning the extreme event statistics, we show evidence that solar power is more volatile than wind power.

DY 26: Focus Session: Slow Dynamics in Glasses and Granular Matter I (joint session DY/ CPP/ DF)

The transition into an amorphous solid state is typically accompanied by the observation of slow dynamics. The understanding of such transitions from first principles has seen progress in many of its aspects recently, including nonlinear response, residual stresses, and non-affine deformations. The Focus Session provides an overview of common phenomena and of general concepts in the physical picture of disordered materials. (Organizers M. Sperl and A. Zippelius)

Time: Thursday 9:30–12:30 Location: HÜL 186

Invited Talk DY 26.1 Thu 9:30 HÜL 186

The memory of sand — •Matthieu Wyart — New York University

Complex systems are characterized by an abundance of meta-stable states. To describe such systems statistically, one must understand how states are sampled, a difficult task in general when thermal equilibrium does not apply. This problem arises in various fields of science, and here I will focus on a simple example, sand. Sand can flow until one jammed configuration (among the exponentially many possible ones) is reached. I will argue that these dynamically-accessible configurations are atypical, implying that in its solid phase sand "remembers" that it was flowing just before it jammed. As a consequence, it is stable, but barely so. I will argue that this marginal stability answers long-standing questions both on the solids and liquid phase of granular materials, and will discuss tentatively the applicability of this idea to other systems.

Invited Talk DY 26.2 Thu 10:00 HÜL 186

Complex rheology at the jamming transition: shear thickening, shear thinning, shear banding — •Claus Heussinger — Institut für theoretische Physik, Universität Göttingen

The jamming paradigm aims at providing a unified view for the elastic and rheological properties of materials as different as foams, emulsions, suspensions or granular media. The usefulness of such a unifying concept hinges on the presence or absence of phenomena that are in some sense *universal*.

In this contribution, we discuss how certain features in the particle interactions affect the rheological properties of the material. First, we discuss the effect of frictional forces, and show how the jamming phase diagram has to be modified as compared to the frictionless scenario [1,2]. Essential findings are a discontinuous and hysteretic jamming transition, as well as a shear thickening regime where frictionless particles are generically shear thinning.

Secondly, we investigate the role of attractive interactions between the particles [3]. For weakly attractive systems a fragile solid develops which displays self-organization towards a minimal (isostatic) connectivity. Moreover, the measured flow curves have unstable regimes, which lead to persistent shearbanding. These features are rationalized by establishing a link between rheology and inter-particle connectivity, which also provides a minimal theoretical model to describe the flow curves.

[1] CH, PRE (2013). [2] M. Grob. CH, A. Zippelius, arXiv (2013). [3] E. Irani, P. Chaudhuri, CH, arXiv (2013).

DY 26.3 Thu 10:30 HÜL 186

Stress-birefringence information in three-dimensional binary granular packings — •Peidong Yu, Stefan Frank-Richter, and Matthias Sperl — Institut für Material Physik im Weltraum, Köln, Deutschland

We report our newly developed 3D stress-birefringence technique and its application in a binary static packing. We show how we precisely determine the stress state of one single spherical particle from its stress-birefringent response to external contacts. Such particles of two different sizes are used in a dense packing with different packing fractions. Based on the knowledge of one-particle calibration, we are able to define a transition point from the integrated stress-birefringent signal of the whole packing under changing packing fraction. Variations of these transition points with different size ratio and specie number ratio of the two particle species are measured and discussed.

DY 26.4 Thu 10:45 HÜL 186

Jamming of Frictional Particles: a First Order Phase Transition — •Matthias Grob[1], Claus Heussinger[2], and Annette Zippelius[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland — [2]Institut für Theoretische Physik, Universität Göttingen, Göttingen, Deutschland

With numerical simulations, we produce flow curves for dense frictional granular media with features different from the frictionless analog. When the strain rate is controlled and increased, a smooth transition from inertial to plastic flow is observed below a critical volume fraction. Above this packing fraction, the transition becomes discontinuous as a hallmark of friction. Upon an increase of packing fraction, the flow curves show hysteretic behaviour, the emergence of a yield stress and the divergence of the shear viscosity - each at a different packing fraction. All the reported behaviour is reproduced with a simple model for a non-equilibrium first order phase transition. An inherent feature of dense frictional granular rheology is that the transition from flowing to jammed states is reentrant with transient jam-and-flow states in between which are, within the models' framework, metastable flow states.

15 min. break

DY 26.5 Thu 11:15 HÜL 186

Vibrational Masking of Critical Decay in the Early beta-Relaxation Regime of Incoherent Intermediate Scattering Functions in Simulated Glass Forming Ni0.5Zr0.5 — •Helmar Teichler — Institut f. Materialphysik, Univ. Göttingen

Results are presented concerning the origin of discrepancy between mode coupling theory (MCT) prediction for critical decay in the early beta-regime and molecular dynamics (MD) simulation data. The discrepancy is known since long in the literature and is heuristically ascribed to effects of atomic vibrations not fully taken into account in MCT. A proper theoretical treatment is missing so far. Here I present a formally exact framework for analyzing the MD data, which allows deducing the origin of the discrepancy and its quantitative description, and I apply it to MD simulated glass forming Ni0.5Zr0.5. The approach relates incoherent intermediate scattering functions (ISFs) from atomic trajectories, which show the discrepancy, to those from inherent structure (IS), which are in agreement with MCT. Cumulant expansion of the ISFs demonstrates that the discrepancy reflects the vibrational density of states, with minor effect of the Boson peak. The results for Ni0.5Zr0.5 rely on the fact that there are only weak correlations between atomic vibrations and IS relaxation displacements in the beta-regime, and that the essential part of the vibrational displacements distribution acts Gaussian-like.

DY 26.6 Thu 11:30 HÜL 186

Glass Transition of Yukawa Systems: Crossover from Hard Sphere to Soft Sphere Limits — •Anoosheh Yazdi[1], Alexei Ivlev[2], Sergei Khrapak[2], Adam Wysocki[3], Hartmut Löwen[4], and Matthias Sperl[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum fuer Luft- und Raumfahrt, 51147 Köln, Germany — [2]Max-Planck-Institut für extraterrestrische Physik, 85741 Garching, Germany — [3]Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, 52425 Jülich, Germany — [4]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, 85741 Düsseldorf, Germany

The mode-coupling theory for ideal glass transitions (MCT) is applied to the single and double Yukawa potential systems. Glass transition curves are obtained in the full range of two control parameters: the screening parameter κ, which is the inverse screening length, and the interparticle potential strength Γ. With increasing κ along the transition, glass form factors and effective packing fractions undergo a crossover from the one-component plasma (OCP) limit, which resembles a very soft sphere system, to a hard sphere system (HSS). The entire transition diagram can be described by analytical functions. Suprisingly and different from those of other potentials, glass transition curves are found to be shifted but otherwise identical to the

melting curves in the control parameter plane.

DY 26.7 Thu 11:45 HÜL 186

rheology near jamming-the influence of lubrication forces — •MOUMITA MAITI and CLAUS HEUSSINGER — Georg-August University of Goettingen, Goettingen, Germany

The talk discusses the role of different dissipation forces on the rheological properties of highly dense non-Brownian suspensions. The focus is on the random close packing limit ("jamming") where particle motion is limited due to steric volume exclusion. We define a simplified lubrication force where we change the dissipation mechanisms by tuning the range of the interaction. Two densities are considered, one is near jamming the other further away. For both densities, a crossover is seen from 'inertia' dominated flow to viscous flow by changing the lubrication range. Interestingly, we observe that velocity fluctuations are independent of the different dissipation mechanisms ("universal")near jamming. Away from jamming this universality is lost and an unexpected non-monotonic dependence is seen. We present an understanding of our findings in terms of geometric constraints of random-close packing and a decoupling of dissipative forces and particle trajectories.

DY 26.8 Thu 12:00 HÜL 186

Lattice Boltzmann Simulations for Glass-Forming Liquids — •SIMON PAPENKORT[1,2] and THOMAS VOIGTMANN[1,2] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Köln, Germany — [2]Zukunftskolleg und Fachbereich Physik, Universität Konstanz, Germany

In continuum mechanics, the Navier-Stokes (NS) equation is used to study fluid flows. The Lattice Boltzmann (LB) model is an efficient method to find solutions of the NS equation of Newtonian liquids even for complex flow geometries.

Complex fluids, such as glass formers, colloidal suspensions, or granular media, display a wide range of non-Newtonian flow effects, determined by the interplay between slow structural dynamics on the microscopic scale, and the mesoscopic flow field. Prominent examples are shear thinning and yield stresses, leading to plug flow in channels.

Starting from first principles, mode coupling theory of the glass transition is able to provide constitutive equations that describe the history effects determining the flow of glass-forming fluids. We present results from a new LB scheme that allows to include memory-integral effects in fluid-mechanics simulations.

DY 26.9 Thu 12:15 HÜL 186

Slow convection in densely packed granular mixtures — •FRANK RIETZ and RALF STANNARIUS — University of Magdeburg, Institute of Experimental Physics, Department of Nonlinear Phenomena

Handling of granulate in partly filled rotating containers is a common situation in industrial processes. Contrary to ensembles of loosely packed grains, the container can be filled so dense that fluidization is limited to a shallow surface layer. Then, the deeper layers are in a locked state, only creeping motions on longer time scales are possible.

We study such a situation in a flat rotating container of aspect ratio 1 that is almost completely filled with a bidisperse mixture. Irrespective of the limited mobility of the grains we observe nonuniform segregation patterns accompanied by slow convective motion. Many features of the convection flow amplitude, like regular oscillatory modulations of the convection velocity, cessations and spontaneous reversals of the circulation are comparable to convection in ordinary liquids at high Rayleigh numbers, in geometries with aspect ratio 1.

[1] F. Rietz & R. Stannarius, Phys. Rev. Lett. 108, 118001 (2012).

DY 27: Nonlinear Dynamics, Synchronization and Chaos - Part II

Time: Thursday 9:30–12:00 Location: ZEU 160

DY 27.1 Thu 9:30 ZEU 160

Scaling of Chaos in Strongly Nonlinear Lattices — •MARIO MULANSKY — Max-Planck-Institut für die Physik komplexer Systeme, Dresden

Although it is now understood that chaos in complex classical systems is the foundation of thermodynamic behavior, the detailed relations between the microscopic properties of the chaotic dynamics and the macroscopic thermodynamic observations still remain mostly in the dark. In this work, we numerically analyze the probability of chaos in strongly nonlinear Hamiltonian systems and find different scaling properties depending on the nonlinear structure of the model. We argue that these different scaling laws of chaos have definite consequences for the macroscopic diffusive behavior, as chaos is the microscopic mechanism of diffusion. This is compared with previous results on chaotic diffusion [New J. Phys. 15, 053015 (2013)], and a relation between microscopic chaos and macroscopic diffusion is established.

DY 27.2 Thu 9:45 ZEU 160

Instability of Velocity-Verlet Integrator as Stochastic Process — •LOTHAR BRENDEL — Universität Duisburg-Essen

The Velocity-Verlet integrator is ubiquitous in simulations of classical many-body systems. Though being time symmetric, it is known to be stable "only" on exponentially long times. We model its loss of stability as a stochastic process and compare the resulting characteristics to actual simulations at the verge of stability.

DY 27.3 Thu 10:00 ZEU 160

"Beating" beats "Mixing" in Heterodyne Detection Schemes — •GERARD J. VERBIEST[1] and MARCEL J. ROST[2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

Heterodyne detection schemes are widely used, as one can measure extremely high-frequencies signals that are otherwise difficult, or even impossible, to measure experimentally. A heterodyne detection scheme can down-convert a high-frequency signal to a lower, easily measurable frequency by mixing it with a reference signal. In general, *beating* and *mixing* are contrary effects: *beating* occurs with a linear interaction, whereas heterodyne *mixing* occurs, if the interaction is nonlinear. Therefore, *beating* is ought to be unimportant in heterodyne schemes, as it does not generate a *mixing* signal. In contrast to this, we show via a derivation of a general analytical model [1] that both *beating* and *mixing* are necessary to explain the generation of the heterodyne signal. *Beating* even dominates the heterodyne signal generated by *mixing*, if the nonlinearity of the system is of higher order than quadratic. Standard textbook equations fail in this case, as they are usually based on second order approximations. We confirm our results with both an experiment [2] and a full numerical calculation [3] on the example of Heterodyne Force Microscopy.

[1] G.J. Verbiest, and M.J. Rost, Nature Physics submitted
[2] G.J. Verbiest et al., Nanotechnology 24, 365701 (2013)
[3] G.J. Verbiest et al., Ultramicroscopy 135, 113 (2013)

DY 27.4 Thu 10:15 ZEU 160

Efficiency of Monte Carlo Methods in Chaotic Systems — •JORGE C. LEITÃO[1], JOÃO P. V. LOPES[2], and EDUARDO G. ALTMANN[1] — [1]Max Planck Institute for The Physics of Complex Systems, Dresden, Germany — [2]Faculdade de Engenharia da Universidade do Porto, Porto, Portugal

Monte Carlo techniques have the potential of dramatically improving the efficiency of simulations of chaotic systems. However, in it is often unclear to which extent an improvement over uniform sampling simulations is actually achieved because the Monte Carlo method struggles to efficiently sample the relevant trajectories of the phase space (e.g., the simulation suffers from critical slowing down). In this talk we discuss the efficiency of different Monte Carlo methods applied to the problem of computing: 1. the distribution of finite-time Lyapunov exponents; and 2. the escape rate in scattering systems.

DY 27.5 Thu 10:30 ZEU 160

Magnetic Spatial Forcing of a Ferrofluid Layer — •FLORIAN MAIER, INGO REHBERG, and REINHARD RICHTER — Experimentalphysik 5, Universität Bayreuth, D-95444 Bayreuth

In isotropic two-dimensional pattern-forming systems with broken up-down symmetry, hexagons are the first pattern to arise due to a transcritical bifurcation, as summarized in [1]. One famous example is the

Rosensweig instability at an interface between ferrofluid and air subjected to a normal magnetic field [2]. However, stripes become the preferred pattern for a spatially periodic resonant forcing [1]. Experiments have been performed using a thin layer of ferrofluid forced by means of a one-dimensional array of current carrying wires [3] with $k_m = k_c$. Here k_m (k_c) denotes the modulation (capillary) wave number, respectively. We report new results for a larger aspect ratio, taking also into account a varying layer thickness.

[1] R. Peter, M. Hilt, F. Ziebert, J. Bammert, C. Erlenkämper, N. Lorscheid, C. Weitenberg, A. Winter, M. Hammele, and W. Zimmermann, Phys Rev. E, **71**, 046212 (2005).

[2] M. D. Cowley and R. E. Rosensweig, J. Fluid Mech., vol. **30**, no. 4, pp. 671-688 (1967).

[3] Th. Friedrich, A. Lange, I. Rehberg, R. Richter, Magnetohydrodynamics, Vol. **47**, No. 2, pp. 167-173 (2011).

15 min break

DY 27.6 Thu 11:00 ZEU 160

Periodically driven oscillatory demixing — •Martin Rohloff[1,2], Julian Vogel[1,2], and Jürgen Vollmer[1,2] — [1]Max Planck Institute for Dynamics and Self-Organisation (MPIDS), 37077 Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, 37077 Göttingen, Germany

Demixing of multiphase fluids with a constant supply of supersaturation can give rise to episodic precipitation of potentially catastrophic impact: geysers, lake outbreaks, volcano eruptions and tropical rain. In all these processes the frequency of this oscillatory demixing is a function of the intensity of the continuous supply. Often, however, convection leads to a periodic modulation of the supply.

Here we present a lab experiment in which repeated precipitation cycles can be observed: A binary liquid mixture that undergoes oscillatory demixing when subjected to a shallow temperature ramp [1]. We perform turbidity measurements to determine the period of the precipitation cycles. Depending on amplitude and frequency of the supply we observe synchronization as well as conditions where only the average supersaturation supply rate is important.

[1] Lapp, T., M. Rohloff, J. Vollmer, B. Hof, 2012 Exp. Fluids 52, 1187

DY 27.7 Thu 11:15 ZEU 160

Chaotic and statistical properties of two coupled Pomeau-Manneville maps — •Matteo Sala[1], Cesar Manchein[2], and Roberto Artuso[3] — [1]MPI PKS, Dynamical systems and Social Dynamics, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Departamento de Física, Universidade do Estado de Santa Catarina, 89219-710 Joinville, Brazil — [3]Center for Nonlinear and Complex Systems, Dipartimento di Scienza ed Alta Tecnologia, Via Valleggio 11, 22100 Como, Italia

By considering a 2-D map on the torus defined by two identical Pomeau-Manneville maps interacting through a linear coupling, we study the subtle interplay between *intermittency* (due to the marginal instability) and *synchronization* (due to the coupling). In particular, we focus on the weak coupling regime in the range of nonlinearity for which the 1-D Pomeau-Manneville map admits an absolutely continuous invariant measure. Our analysis is based on the phase-space *filling rate* of non-synchronized orbits and the associated statistics of both the *recurrence times* and the *finite-time Lyapunov exponents*. Two main results show up: *i*) the detection of a clear stretched-exponential trend in both the phase-space filling rate and the decay of rare values probability for the Lyapunov exponent and *ii*) the coexistence of regular and anomalous behavior in the cumulative probability of recurrence times. These points lead to the conclusion that even a linear, very weak interaction between nonlinear intermittent systems can bring into play extremely non-trivial dynamical features.

DY 27.8 Thu 11:30 ZEU 160

Characterisation of slow cardiovascular oscillations by synchronisation techniques — •Kathrin Dabelow[1], Jan W. Kantelhardt[1], Alexander Müller[2], Petra Barthel[2], and Georg Schmidt[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Medizinische Klinik und Deutsches Herzzentrum der Technischen Universität München

Variations of human heart rate and blood pressure, i. e. cardiovascular oscillations, naturally occur in the high-frequency (HF) regime due to influences of the repiratory process. Also at lower frequencies (LF regime) variations can be found but the specific underlying mechanisms are still subject to discussion. We study the phase synchronisation properties of heart rate and blood pressure time series. Firstly, we decompose the frequency spectrum of cardiovascular signals into overlapping bands of logarithmically equal width. Within each band the synchronisation of the signal with a time-shifted copy, as well as the synchronisation between different signals is analysed in order to determine differences between the HF and LF range. In addition, the prognostic power of these methods is evaluated in patients that survived a myocardial infarction.

DY 27.9 Thu 11:45 ZEU 160

Unveiling generalized synchronization among coupled oscillators and geophysical signals: A recurrence perspective — •Reik V. Donner[1,2], Jan H. Feldhoff[2,3], and Jonathan F. Donges[2,4] — [1]Max Planck Institute for Biogeochemistry, Jena, Germany — [2]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [3]Department of Physics, Humboldt University, Berlin, Germany — [4]Stockholm Resilience Centre, Stockholm University, Sweden

The emergence of complex synchronization phenomena is a characteristic feature of many nonlinear systems. Among other types, generalized synchronization (GS) describes the mutual locking of the different dynamical degrees of freedom in the most general sense. As a consequence, GS is not necessarily reflected in a simple functional interdependence between the variables of two systems, which makes its detection from time series a challenging task. Here, we introduce a set of new indicators of GS based on the concept of recurrences in phase space. Numerical results for two coupled Rössler systems in different dynamical regimes reveal that indicators utilizing recurrence network transitivity as a proxy for the effective dimensionality of the system under study exhibit a particularly good performance in detecting the known transition to GS from short time series data. The corresponding potentials for the analysis of real-world data are exemplified using some time series reflecting climate and ecosystem variability.

DY 28: Extreme Events

Time: Thursday 9:30–12:15 Location: ZEU 146

DY 28.1 Thu 9:30 ZEU 146

Branching in Tsunami Waves — •Henri-Philippe Degueldre[1,2], Jakob J. Metzger[1,2], Ragnar Fleischmann[1], and Theo Geisel[1,2] — [1]MPIDS, am Fassberg 17, 37077 Goettingen, Germany — [2]Institute for Nonlinear Dynamics, Departement of Physics, University of Goettingen, Germany

Branched flow is a universal phenomenon occuring in particle or wave flows propagating through weakly scattering, correlated, random media. Even for very weak disorder in the medium it can lead to extremely strong fluctuations in the wave intensity. We show how tsunami waves are affected by branching. We model the tsunamis propagating over the ocean floor with its complex height fluctuations by the linearized shallow water wave equations with random bathymetries. We calculate the typical distance from the source at which the strongest wave fluctuations occur as a function of the statistical properties of the bathymetry.

DY 28.2 Thu 9:45 ZEU 146

Experimental Observation of a Fundamental Length Scale of Waves in Random Media — •Sonja Barkhofen[5,1], Jakob Metzger[2,3], Ragnar Fleischmann[2], Ulrich Kuhl[4,1], and Hans-Jürgen Stöckmann[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany — [2]Max-Planck-Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [3]Institute for Nonlinear Dynamics, Department of Physics, University of Göttingen, 37077 Göttingen, Germany — [4]LPMC, CNRS UMR 7336, Université de Nice Sophia-Antipolis, F-06108 Nice, France — [5]Applied Physics, University of Paderborn, Warburger Straße 100, 33098 Paderborn, Germany

Waves propagating through a weakly scattering random medium show a pronounced branching of the flow accompanied by the formation of freak waves, i.e. extremely intense waves. Theory predicts that this strong fluctuation regime is accompanied by its own fundamental length scale of transport in random media, parametrically different from the mean free path or the localization length. We report the experimental observation of this scaling using microwave transport experiments in quasi-two dimensional resonators with randomly distributed weak scatterers. Remarkably, the scaling range extends much further than expected from random caustics statistics.

DY 28.3 Thu 10:00 ZEU 146

Statistics of Extreme Waves in Random Media — •Jakob Metzger[1,2], Ragnar Fleischmann[1], and Theo Geisel[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland — [2]Institut für Nichtlineare Dynamik, Universität Göttingen, Deutschland

Waves traveling through random media exhibit random focusing that leads to extremely high wave intensities even in the absence of nonlinearities. Although such extreme events are present in a wide variety of physical systems and the statistics of the highest waves is important for their analysis and forecast, it remains poorly understood in particular in the regime where the waves are highest. We suggest a new approach that greatly simplifies the mathematical analysis and calculate the scaling and the distribution of the highest waves valid for a wide range of parameters [1].

[1] JJ Metzger, R Fleischmann, T Geisel, arXiv:1311.4578

DY 28.4 Thu 10:15 ZEU 146

Optimizing cluster analysis by stochastic methods — •Philip Rinn[1], Yuriy Stepanov[2], Thomas Guhr[2], Joachim Peinke[1], and Rudi Schäfer[2] — [1]ForWind – Center for Wind Energy Research, Institute of Physics, University of Oldenburg, Germany — [2]Faculty of Physics, University of Duisburg-Essen, Germany

A new method to analyze the the results of a clustering algorithm is presented. Using a similarity measure daily prices of S&P 500 stocks are clustered with a top-down clustering scheme to represent states in the financial market. Time series of the distance between each data point and the cluster centers are calculated which describe the evolution of the financial market seen from the respective cluster center.

With methods from stochastic data analysis we separate the stochastic part from the deterministic part of the given time series. From the deterministic part we calculate a potential and find the fixed points of the system. We link the stable fixed points of the deterministic potential to the centers of the aforementioned clusters. Fixed points of the system that do not match with cluster centers can be identified as artificial clusters and ideas for optimizing the clustering to match the systems fixed points can be derived.

DY 28.5 Thu 10:30 ZEU 146

Improving Predictions using the Crooks Fluctuation Theorem — •Julia Gundermann[1], Stefan Siegert[2], and Holger Kantz[1] — [1]Max Planck Institut für Physik komplexer Systeme, Dresden, Germany — [2]University of Exeter, United Kingdom

The Crooks fluctuation theorem is a relation from non-equilibrium thermodynamics, quantifying the amount of work produced in a process more exactly than the second law inequality by giving an exact equation for the work's distribution.

We take this equation as a constraint for the distribution of a random variable and ask the question: Given a finite data set drawn from such a distribution, how can we improve the estimate of this variable to exceed a certain threshold compared to the event frequency deduced from the data set? Using the knowledge about Crooks' relation we propose a forecast that will prove to be "better" than simple counting on the data set. We measure the notion of "better" in terms of the Brier score. Studies of parameters such as exceedance threshold and data set size are presented.

15 min break

DY 28.6 Thu 11:00 ZEU 146

Extreme risks in financial markets - a random matrix approach — Thilo Schmitt, Desislava Chetalova, •Rudi Schäfer, and Thomas Guhr — Fakultät für Physik, Universität Duisburg-Essen

The instability of the financial system as experienced in recent years and in previous periods is often linked to credit defaults, i.e., to the failure of obligors to make promised payments. Given the large number of credit contracts, this problem is amenable to be treated with approaches developed in statistical physics. We introduce the idea of ensemble averaging and thereby uncover generic features of credit risk. We then show that the often advertised concept of diversification, i.e., reducing the risk by distributing it, is deeply flawed when it comes to credit risk. The risk of extreme losses remain due to the ever present correlations, implying a substantial and persistent intrinsic danger to the financial system.

DY 28.7 Thu 11:15 ZEU 146

Mapping the dynamics of quantiles in climate change relevant observables — •Sandra Chapman[1,2,3], David Stainforth[4,1,5], and Nicholas Watkins[2,4,1,6] — [1]CFSA, Physics, Univ. of Warwick, UK — [2]MPIPKS, Dresden, Germany — [3]Mathematics and Statistics, UIT, Norway — [4]LSE London, UK — [5]Environmental Change Institute, Univ. of Oxford, UK — [6]MCT, Open Univ., Milton Keynes, UK

Climate change poses challenges for decision makers across society, not just in preparing for the climate of the future but even when planning for the climate of the present day. When making climate sensitive decisions, policy makers and adaptation planners would benefit from information on local scales and for user-specific quantiles (e.g. the hottest/coldest 5% of days) and thresholds (e.g. days above 28 C), not just mean changes. Here, we translate observations of weather (daily records of temperature and precipitation) into observations of climate change, providing maps of the changing shape of climatic distributions. We have developed a simple deconstruction of how the difference between the cumulative density function of a weather observable from two different time periods can be assigned to the combination of natural statistical variability and/or the consequences of secular climate change; this also relates to the dynamics of return times. We will relate this to the dynamics of exceedence above a threshold.

DY 28.8 Thu 11:30 ZEU 146

Prediction of extreme temperatures: The issue of the performance measure — •Holger Kantz[1] and Stefan Siegert[2] — [1]MPI for the Physics of Complex System, Germany — [2]University of Exeter, UK

The perceived performance of every prediction scheme depends of the way how performance is measured. We compare different such performance measures on predictions of extreme temperature anomalies, using different forecast models. The embarrassing result is that not only quantitative details of performance but even the ranking of our four different models depends on the scoring scheme used, so that the notion of "the best forecast method" becomes very questionable.

DY 28.9 Thu 11:45 ZEU 146

Predictors and Prediction Mechanisms of Extreme Events in Spatio Temporal Chaotic systems — •Nahal Sharafi[1], Sarah Hallerberg[1], and Marc Timme[1,2,3] — [1]Network Dynamics, Max Planck Institute for Dynamics and Self-Organization (MPIDS), D-37077 Göttingen, Germany — [2]Faculty of Physics, University of Göttingen, D-37077 Göttingen, Germany — [3]Bernstein Center for Computational Neuroscience, D-37077 Göttingen, Germany

Extreme events happen in a variety of dynamical systems. Marked by their high magnitude as well as their infrequent and irregular occurrence they can lead to disasters. Employing quantifiers of chaos we work towards identifying changes in the dynamical structure of complex, high-dimensional systems before an extreme event happens and use them as precursors of extreme events. As candiate precursors, we consider changes in different features of covariant Lyapunov vectors such as growth rate, localization, direction etc. before an extreme event happens in prototypes of chaotic systems. Apart from possible practical implementations, such as predictions, we use the relation between predictor and event in order to understand the dynamical origins of the events under study. For the Lorenz 1996 model, a paradigmatic model for high-dimensional chaotic systems, we computed covariant Lyapunov vectors and identified features of these vectors that indicate extreme events.

DY 28.10 Thu 12:00 ZEU 146

On the surprising robustness of the surplus run length ratio formula, and its application to extreme bursts in time series from natural complex systems — •Nicholas Watkins[1,2,3,4], Sandra Chapman[1,2,5], and Philip Hush[2] — [1]MPIPKS, Dresden, Germany — [2]CFSA, Physics, University of Warwick, Coventry, UK — [3]MCT, Open University, Milton Keynes, UK — [4]CATS, LSE, London, UK — [5]Maths and Statistics, UIT, Tromso, Norway

"Bursts", events that begin when a time series exceeds a threshold u, and end when it drops below it, have been widely studied in models of intermittent dynamical systems such as SOC and turbulence, and in natural datasets. Analytical approaches to bursts are needed which permit handling time dependence and heavy tailed amplitudes, and make contact with mature mathematics such as the theory of random fields and level crossings. We will discuss one such technique, which we call the surplus run length ratio [SRLR] formula, which states that the expectation value of the time T_u between successive up and downcrossings of a threshold u by values of stationary time series from a stochastic process $X(t)$ is the empirical survival function of X divided by the time rate of upcrossings at that level [Volkonskii, 1960; Cramér and Leadbetter,1967; Lawrance and Kottegoda, 1977]. We show that the SRLR formula applies surprisingly widely in highly skewed (log-normal), heavy tailed (α-stable) and long range dependent (fractional Gaussian) cases, among others. We demonstrate its utility on a non-Gaussian, correlated, natural example which has been previously studied using bursts, the auroral electrojet AE ionospheric index.

DY 29: Symposium SYCP: The Collapsed State of Polymers: From Physical Concepts to Applications and Biological Systems (joint session CPP, BP,DY)

Time: Thursday 9:30–12:15 Location: HSZ 02

Invited Talk DY 29.1 Thu 9:30 HSZ 02

Why do polymer collapse and polymer topology frustrate each other — •Alexander Y. Grosberg — Department of Physics and Center for Soft Matter Research, New York University, NY, USA

Polymer topology is most commonly studied in the context of a melt or concentrated solution. Here, the role of topological constraints is discussed in the context of a single chain swelling or collapse behavior, both in kinetics and in equilibrium (the latter in case topology is quenched, one way or another). Biological aspects are discussed in the context of both chromatin and proteins.

Invited Talk DY 29.2 Thu 10:00 HSZ 02

Nanoscopy of nuclear Genome Structure — •Christoph Cremer — Institute of Molecular Biology (IMB), D-55128 Mainz — Kirchhoff-Institute of Physics (KIP) University Heidelberg, D-69120 Heidelberg — Institute of Pharmacy and Molecular Biotechnology (IPMB) University Heidelberg, D-69120 Heidelberg

Numerical models as well biochemical data indicate a decisive functional role of genome nanostructure; but due to the conventional resolution limits of far-field light microscopy, direct light microscopic tests of such models were believed to be impossible. However, novel developments in optical technology and photophysics succeeded to radically overcome these conventional limits. With such"superresolution" techniques, it has become possible to analyze nuclear genome structure with a greatly enhanced light optical resolution down to a few tens of nanometer. Application examples will be presented on the use of such "nanoscopy" procedures to measure in cell nuclei the size of individual small chromatin domains, of replication and transcription complexes, as well as the spatial distribution of individual nuclear proteins and of short specifically labelled DNA sequences. It is anticipated that the wealth of nanoscale information on nuclear genome nanostructure accessible by the novel superresolution approaches will substantially contribute to the theoretical understanding of the folding in space and time of the huge polymers called chromosomes, and its functional consequences.

Invited Talk DY 29.3 Thu 10:30 HSZ 02

Blood Clotting Inspired Polymer Physics — •Alfredo Alexander-Katz — Massachusetts Institute of Technology

Nature has devised creative and efficient ways of solving complex problems, and one of these problems is that of blood clotting in flowing conditions. In fact, nature has used a novel combination of polymer physics and chemistry that enhances the self-healing propensity of a vessel when strong flows are present while avoiding coagulation when the flow is diminished, a rather counter-intuitive phenomenon. Underlying this process is a globular biopolymer, the so-called von Willebrand Factor, whose function is strongly regulated by flow. In this talk I will present our work on this macromolecule starting from the single molecule approach and building up to the multi component system that more closely resembles blood. I will emphasize how new concepts have emerged from trying to understand such a complex system, in particular I will show how these polymers can display giant non-monotonic response to shear, as well as a very large propensity to form polymer-colloid composites in flow while being a stable dispersed suspension in quiescent conditions. In fact, the aggregation behavior is universal and can be explained with simple scaling arguments. These novel concepts and results are in principle not unique to blood clotting and can have important ramifications in other areas.

15 min. break

Invited Talk DY 29.4 Thu 11:15 HSZ 02

Modeling dynamic spatial genome organization in yeast — •Christophe Zimmer — Institut Pasteur, 25 rue du Docteur Roux, 75015 Paris

The spatial organization and dynamics of chromosomes plays important roles for gene expression, DNA repair and replication, but its underlying principles remain poorly known. We will present quantitative experimental data and simulation results showing that the territorial organization the interphase yeast nucleus and the dynamics of chromosomes can be largely predicted by a model based on generic polymer physics with a minimal set of DNA sequence-specific constraints and assumptions. We will also discuss extensions of our budding yeast model to other organisms and address implications of this model for a quantitative understanding of DNA repair.

Invited Talk DY 29.5 Thu 11:45 HSZ 02

Ring polymers in the melt state: the physics of crumpling —

•Ralf Everaers[1] and Angelo Rosa[2] — [1]Laboratoire de Physique et Centre Blaise Pascal, ENS Lyon, CNRS UMR5672, 46 allée d'Italie, 69364 Lyon, France — [2]SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste (Italy)

The conformational statistics of ring polymers in melts or dense solutions is strongly affected by their quenched microscopic topological state. The effect is particularly strong for non-concatenated unknotted rings, which are known to crumple and segregate and which have been implicated as models for the generic behavior of interphase chromosomes. Here we use a computationally efficient multi-scale approach to identify the subtle physics underlying their behavior, where we combine massive Molecular Dynamics simulations on the fiber level with Monte Carlo simulations of a wide range of lattice models for the large scale structure. We show that (i) topological constraints may be neglected on scales below the standard entanglement length, L_e, (ii) that rings with a size $1 \leq L_r/L_e \leq 30$ exhibit nearly ideal lattice animal behavior characterized by primitive paths which are randomly branched on the entanglement scale, (iii) that larger rings are weakly swollen relative to ideal lattice animals with gyration radii $\langle R_g^2(L_r)\rangle \propto L_r^{2\nu}$ and $\nu \approx 1/d > 1/4$, and (iv) that ring melts can be *quantitatively* mapped to coarse-grained melts of *interacting* randomly branched primitive paths.

DY 30: Graphene-Like Materials: Silicene, MoS_2 and Relatives (joint session HL/DY/DS/MA/O/TT)

Time: Thursday 10:00–12:30 Location: POT 081

DY 30.1 Thu 10:00 POT 081

Many-body effects in 2D hexagonal semimetals and semiconductors — •Tineke Stroucken, Johanna Grönqvist, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps University Marburg, Renthof 5, D-35032 Marburg, Germany

Recently, a variety of graphene-analogues materials like h-BN, silicene or transition-metal dichalcogenides have been fabricated. Similar to graphene, these novel material systems display exciting new physical properties, distinct from their bulk counterparts.

Owing to the symmetry of the hexagonal lattice, band edge carriers are described by massive Dirac Fermions. Typically, the Fermi-velocity is in the range of $c/300$ or below. This yields effective fine structure constants $\alpha = e^2/\epsilon\hbar v_F \gtrsim 2/\epsilon$, implying prominent Coulomb interaction and relativistic effects. Particularly, $\alpha \gtrsim 1$ indicates an excitonic instability of the noninteracting ground state.

In this presentation, we discuss conditions for strong Coulomb coupling in 2D hexagonal crystals and identify experimentally observable signatures signaling an excitonic ground state. To this end, the gap equations are solved self consistently with the polarization function, which depends on the interacting band structure.

[1] T. Stroucken *et al.*, Phys. Rev. B 84, 205445 (2011)
[2] J. H. Grönqvist *et al.*, EPJ B 85, 12 (2012)
[3] T. Stroucken *et al.*, Phys. Rev. B. 87, 245428(2013)
[4] T. Stroucken *et al.*, Appl. Phys. Lett. 103, 163103 (2013)

DY 30.2 Thu 10:15 POT 081

Single and Multi-Layer Silicene: Growth, Properties and Perspectives — •Patrick Vogt[1], Thomas Bruhn[1], Andrea Resta[2], Paola De Padova[3], and Guy Le Lay[2] — [1]Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Aix-Marseille University, CNRS- PIIM UMR 7345, F-13397 Marseille Cedex 20, France — [3]Instituto di Struttura della Materia, Consiglio Nazionale delle Ricerche -ISM, via Fosso del Cavaliere, 00133 Roma, Italy

Silicene, a new silicon allotrope with a graphene-like honeycomb structure, has recently attracted considerable interest, because its topology confers to it the same remarkable electronic properties as those of graphene, with the potential advantage of being easily integrated in current Si-based nano/micro-electronics offering novel technological applications.

We will discuss the epitaxial formation of single layer silicene on Ag substrates and its structural and electronic properties [1-2]. Based on these results we will look at the growth of silicene multi-layers which can be explained by stacking of single silicene sheets [3-4]. Different experimental techniques are used to investigate atomic structure and electronic properties of this layered system and to discuss its similarities to graphite.

1) Vogt, P. et al., Phys. Rev. Lett. 108, 155501 (2012).
2) Avila, J. et al., J. Phys.: Condens. Matter 25, 262001 (2013).
3) De Padova, P.; Vogt, et al. Appl. Phys. Lett. 102, 163106 (2013).
4) Resta, A. et al., Sci. Rep. 3, 2399 (2013).

DY 30.3 Thu 10:30 POT 081

Optical and vibrational properties of MoS2 — •Ludger Wirtz[1], Alejandro Molina-Sanchez[1], and Kerstin Hummer[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg — [2]Faculty of Physics, University of Vienna, Austria

Monolayer MoS2 is currently receiving a lot of attention as a potential alternative to graphene. Its band gap of about 2eV (depending on the dielectric environment) makes it a suitable candidate for thin-film electronics. The optical and vibrational properties of mono-layer, few-layer, and bulk are seemingly straightforward to calculate. Nevertheless some surprises occur: the phonon dispersion displays an anomalous Davydov splitting and the optical absorption spectra display a rich structure of excitonic peaks in the band-gap and in the continuum of interband transitions. We give a short review of the state-of-the art and discuss recent advances in the understanding of the influence of the substrate on the vibrations and electronic excitations.

DY 30.4 Thu 10:45 POT 081

Carrier- and valley dynamics of singlelayer MoS_2 — •Gerd Plechinger[1], John Mann[2], Christian Schüller[1], Ludwig Bartels[2], and Tobias Korn[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Chemistry, Physics, and Materials Science and Engineering, University of California, CA 92521 Riverside, USA

Consisting of an only 0.7 nm thin S-Mo-S sheet and offering a direct bandgap at the K-points in the Brillouin zone, singlelayer MoS_2 represents a promising semiconductor material for flexible and transparent optoelectronic applications. By means of chemical vapor deposition (CVD), large-area films (several mm^2) of singlelayer MoS_2 can be produced. These were characterised by photoluminescence and Raman spectroscopy. In order to investigate the carrier dynamics, we performed pump-probe measurements in the spectral range of the optical transitions in singelayer MoS_2. Helicity-resolved PL measurements have demonstrated an efficient valley polarisation of the K^+ or K^- valley at near-resonant excitation. We probe these valley dynamics with Kerr spectroscopy and find a biexponential decay of the valley polarisation with decay times of a few tens of ps and a few hundreds of ps at low temperatures.

Coffee break (15 min.)

DY 30.5 Thu 11:15 POT 081

Photocurrent studies on semiconducting MoS2 — Marina Hoheneder, •Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching

The current interest in transition metal dichalcogenides is stimulated by their peculiar electrical and optoelectrical properties and their potential for novel device applications. We investigate the semiconductor MoS2, which shows a crossover from an indirect to a direct bandgap semiconductor by thinning it down to a monolayer. We prepare MoS2 samples through micromechanical exfoliation and characterize the thin flakes with Raman spectroscopy. We further study photocurrent generation of single and few layer MoS2 in dependence of wavelength and power of the exciting light. We gratefully acknowledge financial support by BaCaTec.

DY 30.6 Thu 11:30 POT 081

Resonant Inelastic Light Scattering on MoS_2 — •Bastian Miller, Eric Parzinger, Alexander Holleitner, and Ursula Wurstbauer — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garch-

ing (Germany)

Two-dimensional layered 'van-der Waals' materials are of increasing interest for fundamental research due to their peculiar band-structure.

We utilize inelastic light scattering - a contactless and extremely versatile tool - to study phonon excitation spectra of mono- and fewlayer MoS_2. The phonon modes are unique fingerprints of the material properties and are sensitive to defects, strain, doping and the number of MoS_2 -layers.

We observe signatures of multistep scattering processes involving phonon-phonon, electron-phonon as well as electronic excitations under resonant conditions, where the incoming or outgoing light meets the energy of a fundamental optical transition of the system.

DY 30.7 Thu 11:45 POT 081

The effect of substrate and environment on the elementary excitations of MoS_2 — •Eric Parzinger[1], Marina Hoheneder[1], Bastian Miller[1], Anna Cattani-Scholz[1], Alexander Holleitner[1], Joel W. Ager[2], and Ursula Wurstbauer[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, 85748 Garching (Germany) — [2]Joint Center for Artificial Photosynthesis, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley, California 94702 (United States)

The novel two-dimensional layered 'van-der Waals' material Molybdenum disulfide (MoS_2) is investigated using inelastic and resonant light scattering - a contactless and extremely versatile tool - to study phonon and electronic excitations. In particular, we focus on the influence of different supporting materials (SiO_2, sapphire and SAMs of organic molecules) as well as various environmental conditions (ambient, vacuum and water) on the low energy excitations of MoS_2. We find that both, different substrate and environment give rise to a significant modification of the most prominent Raman modes, whereas a monolayer is most effected by the environmental conditions. We gratefully acknowledge financial support by BaCaTec.

DY 30.8 Thu 12:00 POT 081

Spin-orbit coupling, quantum dots, and qubits in transition metal dichalcogenides — •Andor Kormanyos[1], Viktor Zolyomi[2], Neil Drummond[2], and Guido Burkard[1] — [1]Universität Konstanz — [2]Lancaster University

We derive an effective Hamiltonian describing the dynamics of electrons in the conduction band of transition metal dichalcogenides (TMDC) in the presence of perpendicular electric and magnetic fields. We discuss both the intrinsic and Bychkov-Rashba spin-orbit coupling (SOC) induced by an external electric field. We identify a new term in the Hamiltonian of the Bychkov-Rashba SOC which does not exist in III-V semiconductors. We point out important differences in the spin-split conduction band between different TMDC compounds. A significant consequence of the strong intrinsic SOC is an effective out-of-plane g-factor for the electrons which differs from the free-electron g-factor $g \simeq 2$. Using first-principles calculations, we give estimates of the various parameters appearing in the theory. Finally, we consider quantum dots (QDs) formed in TMDC materials and derive an effective Hamiltonian allowing us to calculate the magnetic field dependence of the bound states in the QDs. We find that all states are both valley and spin split, which suggests that these QDs could be used as valley-spin filters. We explore the possibility of using spin and valley states in TMDCs as quantum bits, and conclude that, due to the relatively strong intrinsic SOC in the conduction band, the most realistic option appears to be a combined spin-valley (Kramers) qubit at low B fields.

DY 30.9 Thu 12:15 POT 081

Analytical approach to excitonic properties of MoS2 — •Gunnar Berghäuser and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We present an analytical investigation of the optical absorption spectrum of monolayer molybdenum disulfide (MoS2). Based on the density matrix formalism [1], our approach gives insights into the microscopic origin of excitonic transitions, their relative oscillator strength, and binding energy [2]. We show analytical expressions for the carrier-light coupling element, which contains the optical selection rules and well describes the valley- selective polarization in MoS2 . In agreement with experimental results, we find the formation of strongly bound electron-hole pairs due to the efficient Coulomb interaction. The absorption spectrum of MoS2 on a silicon substrate features two pronounced peaks at 1.91 eV and 2.05 eV corresponding to the A and B exciton, which are characterized by binding energies of 420 meV and 440 meV, respectively. Our calculations reveal their relative oscillator strength and predict the appearance of further low-intensity excitonic transitions at higher energies. The presented approach is applicable to other transition metal dichalcogenides and can be extended to investigations of trion and biexcitonic effects.

[1] E. Malic and A. Knorr, Graphene and Carbon Nanotubes: Ultrafast Optics and Relaxation Dynamics, 1st ed. (Wiley-VCH, Berlin, 2013).

[2] Gunnar Berghäuser and Ermin Malic, arXiv:1311.1045 (2013)

DY 31: Evolutionary Game Theory and Economic Models (joint session SOE/ BP/ DY)

Time: Thursday 11:00–12:15 Location: GÖR 226

DY 31.1 Thu 11:00 GÖR 226

Learning dynamics explains human behavior in Prisoner's Dilemma on networks — •Giulio Cimini[1] and Angel Sanchez[1,2] — [1]Grupo Interdisciplinar de Sistemas Complejos (GISC), Universidad Carlos III de Madrid, 28911 Leganés, Madrid, Spain — [2]Instituto de Biocomputación y Física de Sistemas Complejos (BIFI), Universidad de Zaragoza, 50018 Zaragoza, Spain

Cooperative behavior lies at the very basis of human societies, yet its evolutionary origin remains a key unsolved puzzle. Whereas reciprocity or conditional cooperation is one of the most prominent mechanisms proposed to explain the emergence of cooperation in social dilemmas, recent experimental findings on networked Prisoner's Dilemma games suggest that conditional cooperation also depends on the previous action of the player—namely on the 'mood' in which the player currently is. Roughly, a majority of people behave as conditional cooperators if they cooperated in the past, while they ignore the context and free-ride with high probability if they did not. However, the ultimate origin of this behavior represents a conundrum itself. Here we aim specifically at providing an evolutionary explanation of moody conditional cooperation. To this end, we perform an extensive analysis of different evolutionary dynamics for players' behavioral traits—ranging from standard processes used in game theory based on payoff comparison to others that include non-economic or social factors. Our results show that only a dynamic built upon reinforcement learning is able to give rise to evolutionarily stable moody conditional cooperation, and at the end to reproduce the human behaviors observed in the experiments.

DY 31.2 Thu 11:15 GÖR 226

Human coordination in the presence of local and global information: A laboratory experiment — •Alberto Antonioni[1,2], Marco Tomassini[1], and Angel Sánchez[2] — [1]University of Lausanne, Switzerland — [2]Universidad Carlos III de Madrid, Spain

Pure coordination games arise in many situations that affect the functioning of society. In fact, many frequent social and economic activities require individuals to coordinate their actions on a common goal since in many cases the best course of action is to conform to the standard behavior. In particular, social coordination can be studied through coordination games between individuals located in space. Here we study the behavior of humans in the laboratory when they play a pure coordination game in a setting in which subjects are situated in a virtual two-dimensional grid space and can move around. We compare a local information setting situation to one in which global information is available. In the local information treatment subjects can see only the eight cells that are their spatial neighbors in the grid and they can decide if they want to move and/or pay a cost to switch to the other strategy type. In the global treatment subjects are in the same condition as before but they possess also the global information about the current fraction of strategies in the population. We observe that in the local information treatment people tend to converge to two separated monomorphic clusters each playing a different strategy. In contrast, in

the global setting this can lead to full predominance of one strategy when strategy fluctuations reach a threshold such that imitation of the majority sets in.

DY 31.3 Thu 11:30 GÖR 226

Differential value of information in non-cooperative games — Nils Bertschinger[1], David H. Wolpert[2], •Eckehard Olbrich[1], and Jürgen Jost[1,2] — [1]Max Planck Institut für Mathematik in den Naturwissenschaften, Leipzig — [2]Santa Fe Institute, NM, USA

We study how players value changes in the information structure of non-cooperative games with imperfect information.

We use the functionals central to Shannon's information theory to quantify amounts of information study how changes in the values of those functionals are related to changes in the expected utility of the players. Our approach is based on the Multi-Agent Influence Diagram representation of games, and is based on a generalization of the concept of marginal utility in decision scenarios to apply to infinitesimal changes of the channel parameters in non-cooperative games. Using that framework we derive general conditions for the possibility of a negative value of information, and show that generically, these conditions hold in all games unless one imposes a priori constraints on the allowed changes to information channels. In other words, in any game in which a player values some aspect of the game's specification beyond the information provided in that game, there will be an infinitesimal change to the parameter vector specifying the game that increases the information but hurts the player.

We demonstrate these results numerically for a leader-follower game and discuss their general implications.

DY 31.4 Thu 11:45 GÖR 226

Stability of Zero-Sum Games in Evolutionary Game Theory — •Johannes Knebel, Torben Krüger, Markus F. Weber, and Erwin Frey — Ludwigs-Maximilians-Universität, München, Deutschland

Evolutionary game theory has evolved into a successful theoretical concept to study mechanisms that govern the evolution of ecological communities. On a mathematical level, this theory was formalized in the framework of the celebrated replicator equations (REs) and its stochastic generalizations.

In our work, we analyze the long-time behavior of the REs for zero-sum games with arbitrarily many strategies, which are generalized versions of the children's game Rock-Paper-Scissors (1). We demonstrate how to determine the strategies that survive and those that become extinct in the long run. Our results show that extinction of strategies is exponentially fast in generic setups, and that conditions for the survival can be formulated in terms of the Pfaffian of the REs' antisymmetric payoff matrix. Consequences for the stochastic dynamics, which arise in finite populations, are reflected by a generalized scaling law for the extinction time in the vicinity of critical reaction rates.

Our findings underline the relevance of zero-sum games as a reference for the analysis of other models in evolutionary game theory.

(1) J. Knebel, T. Krüger, M.F. Weber, E. Frey, Phys. Rev. Lett. 110, 168106 (2013)

DY 31.5 Thu 12:00 GÖR 226

Opportunistic strategies and the emergence of responsible punishment — •Arne Traulsen — Max-Planck-Institute for Evolutionary Biology, Evolutionary Theory Group, Plön, Germany

One way to promote cooperation among selfish actors is to allow for the opportunity to punish those peers who do not cooperate. However, the vast majority of models and behavioral experiments considers situations in which actors cannot assess whether it is likely that they will be punished. If this information is available, opportunistic strategies that act according to this information become possible and lead to the emergence of responsible punishment targeted at non-cooperators only, without the problems of antisocial punishment, second order free-riding or spite. Also for institutional, so called pool punishment, such opportunistic strategies are successful, which implies that the presence of punishment institutions should be made public.

DY 32: Glasses and Glass Transition - Part I (joint session CPP/ DY/DF)

Time: Thursday 11:45–12:45 Location: ZEU 114

Invited Talk DY 32.1 Thu 11:45 ZEU 114

Dynamics and thermodynamics of glassy polymers below the glass transition temperature — •Daniele Cangialosi — Paseo M Lardizabal 5, 20080 San Sebastian, Spain

Glass-forming systems constitute an important class of materials. Among different aspects, the dramatic slowing down of the dynamics when decreasing temperature and the possible connection between such slowing down and the thermodynamics of the glass-former have been intensively studied. It has been speculated that mere extrapolation of the dynamics and thermodynamics to temperatures below the glass transition temperature (T_g) produces a singularity at a finite temperature, with divergent relaxation time and vanishing configurational entropy. Here the dynamics and thermodynamics are studied at temperatures as low as T_g- 40 K by performing enthalpy recovery experiments on glassy polymers for times up to 10^7-10^8 seconds. We find a single stage recovery behavior for temperatures larger than about T_g- 10 K. A double stage recovery is observed for $T < T_g-$ 10 K. The enthalpy recovered after the two-stage decay equals that extrapolated from the melt, whereas partial enthalpy recovery occurs in the first decay. From the analysis of the time to reach each equilibrium it is found that the equilibration time corresponding to the first stage recovery exhibits relatively low activation energy, whereas the second one exhibits activation energy similar to that of the polymer segmental relaxation. These results indicate a complex scenario of the dynamics and thermodynamics below T_g with multiple equilibration steps and leave open the question the finite temperature singularity.

DY 32.2 Thu 12:15 ZEU 114

Excess heat capacity and fictive temperature of polystyrene in a wide range of cooling and heating rates — •Gunnar Schulz[1], Timur Vasilievich Tropin[2], Yeong Zen Chua[1], Jürn W. P. Schmelzer[1], and Christoph Schick[1] — [1]Institut für Physik , AG Polymerphysik, Universität Rostock, Rostock, Germany — [2]Frank Laboratory of Neutron Physics, Joint Institut for Nuclear Research, Dubna, Moscow region, Russia

The physical characteristics of polystyrene allow straightforward and reproducible measurements of heat capacity, C_p, glass transition temperature, T_g, and other properties. The possibility to reuse one sample for numerous cooling and heating cycles permits the investigation of the influence of the cooling and heating rates on C_p and T_g.

In our research, we conduct the cooling phases with various (constant) cooling rates, but the respectively following heating phases with only one heating rate. The comparison of the heat capacities observed after different cooling rates results in an excess C_p, which we also calculate by means of a model.

Our measurements furthermore yield the fictive temperature in the cooling rate range from $10^{-4}\,\mathrm{K\,s^{-1}}$ to $10^{4}\,\mathrm{K\,s^{-1}}$. We compare these results with the dynamic T_g observed by means of temperature-modulated differential scanning calorimetry (TMDSC). The dependence of the fictive T_g on the cooling rate and the dependence of T_g on the modulation frequency turn out to be closely related.

DY 32.3 Thu 12:30 ZEU 114

Glassy dynamics and physical aging in fucose saccharides as studied by Infrared- and Broadband Dielectric Spectroscopy — •Wilhelm Kossack[1], Karolina Adrjanowicz[2], Magdalena Tarnacka[1], Wycliffe Kiprop Kipnusu[1], Mateusz Dulski[2], Emanuel Urandu Mapesa[1], Kamil Kaminski[2], Sebastian Pawlus[2], Marian Paluch[2], and Friedrich Kremer[1] — [1]Universität Leipzig, Linnestr.5, Molekülphysik, 04103 Leipzig, Germany — [2]Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland

Fourier Transform InfraRed (FTIR) and Broadband Dielectric Spectroscopy (BDS) are combined to study both, the intra- and intermolecular dynamics for two isomers of glass forming fucose, far below and above the calorimetric glass transition temperature, T_g. It is shown, that the various IR-active vibrations exhibit in their spectral position and oscillator strength quite different temperature dependen-

cies, proving their specific signature in the course of densification and glass formation. The coupling between intra- and inter-molecular dynamics is exemplified by distinct changes of IR active ring vibrations far above the calorimetric glass transition temperature at about $1.16T_g$, where the dynamic glass transition (α relaxation) and the secondary β relaxation merge. — For samples physically annealed below T_G slower isothermal relaxation times than extrapolated from liquid state are observed .

DY 33: Networks, From Topology to Dynamics - Part II (joint session SOE/ DY/ BP)

Time: Thursday 12:15–13:00 Location: GÖR 226

DY 33.1 Thu 12:15 GÖR 226

Synchronization in two-layer multiplex networks of conformist and contrarian interactions — •Maximilian Sadilek[1] and Stefan Thurner[1,2,3] — [1]Section for Science of Complex Systems, Medical University of Vienna, Spitalgasse 23, A-1090, Austria — [2]Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501, USA — [3]International Institute for Applied Systems Analysis, Schlossplatz 1, A-2361 Laxenburg, Austria

Several mathematical models have been proposed to describe synchronization in social, biological and physical systems, the most known being the Kuramoto model (KM).

We present a Kuramoto-type model on two layers which is designed to capture the interplay of synchronization-enhancing (conformist) and -reducing (contrarian) links in a multiplex network. The model is a combination of a KM on the first layer and a phase shifted KM on the second layer. The topology of the layers varies from random networks to small world networks.

We find indications of a phase transition from the synchronized to the unsynchronized phase in terms of the phase shift parameter of the model. Further, we observe an upward shift of the dominant frequencies in the power spectra with increasing values of the phase shift parameter.

These results may elucidate the understanding of synchronization modes in the human brain and their consequences.

DY 33.2 Thu 12:30 GÖR 226

Controllability of Temporal Networks — •Márton Pósfai[1,2] and Philipp Hövel[2,3] — [1]Department of Physics of Complex Systems, Eötvös University, Budapest, Hungary — [2]Institut für Theoretische Physik, TU Berlin, Berlin, Germany — [3]Bernstein Center for Computational Neuroscience, HU Berlin, Berlin, Germany

The control of complex systems is an ongoing challenge of complexity research. Resent advances making use of structural control made it possible to deduce a wide range of control related properties from the network representation of complex systems. Here we examine the controllability of complex systems for which the timescale of the dynamics we control and the timescale of changes in the network topology are comparable. We provide analytical and computational tools to study the controllability of such systems based on temporal network characteristics of the system. We apply these results to investigate the controllable subnetwork using a single input. We present analytical results for a simple class of temporal network models, and we preform measurements using data collected from real systems. Depending on the density of the interactions compared to the timescale of the dynamics, we witness a phase transition describing the sudden emergence of a giant controllable subspace spanning a finite fraction of the network. We also study the role of temporal patterns in real data making use of various randomization processes, with special focus on the role of the hubs.

DY 33.3 Thu 12:45 GÖR 226

Analysis of local network structure by node-specific triadic Z-score profiles — •Marco Winkler and Jörg Reichardt — Institute for Theoretical Physics, University of Würzburg, Germany

Over the last decade so called network motifs have attracted high attention. A motif is a subgraph pattern that appears significantly more often than in a random network with the same degree distribution as the original one. Triadic Z-score profiles, $\vec{Z}$, assign every possible triadic subgraph pattern i a score Z_i, corresponding to the magnitude of over-/underrepresentation of the pattern compared to the random null model. These Z-score profiles are a common tool to analyze complex networks.

However, triad patterns are not necessarily homogeneously distributed over the network. Therefore, we introduce the concept of *node-specific Z-scores*. For the node-specific Z-score profile, $\vec{Z}^\alpha$, of a node α, only the triads it participates in are taken into account. The node-specific Z-score profiles can then be used for classification of a network's vertices into different structural groups. We present results for various real-world data sets including neural networks and transcription networks.

DY 34: Symposium SYGP: Stochastic Dynamics of Growth Processes in Biological and Social Systems

Time: Thursday 15:00–17:45 Location: HSZ 02

Invited Talk DY 34.1 Thu 15:00 HSZ 02

Noisy invasions: large fluctuations in stochastic invasion models — •Baruch Meerson — Racah Institute of Physics, Hebrew University of Jerusalem, Jerusalem 91904 Israel

Invasion fronts have been recognized as important, and often fateful, phenomena in ecology, epidemiology and biological evolution. The position of an invasion front fluctuates because of the shot noise of individual reactions. What is the probability to observe, at a given time, a front displacement that is considerably smaller or larger than that predicted from deterministic theory? The answer strongly depends on whether the front propagates into a metastable or unstable state, and I will review recent theoretical progress in both cases. The progress is mostly based on a dissipative version of WKB theory which assumes many individuals in the front region. In this theory the most likely history of the system, for a given front displacement, is encoded in a special trajectory of the underlying effective Hamilton mechanics, a classical field theory. This special trajectory is described by a traveling front solution. For fronts, propagating into unstable states, very large front displacements are much more likely than very small ones. The leading contribution to the probability density of a large displacement comes from a few fastest particles running ahead of the front. For such fronts the WKB theory breaks down, and new methods are needed.

Invited Talk DY 34.2 Thu 15:30 HSZ 02

Fractal clustering of inertial particles in random velocity fields — •Bernhard Mehlig and Kristian Gustavsson — Department of Physics, University of Gothenburg, 41296 Gothenburg, Sweden

Independent particles suspended in incompressible turbulent or randomly mixing flows may cluster together even though incompressible flows exhibit no sinks. This is an inertial effect: inertia allows the particles to detach from the flow. Distinct mechanisms have been invoked to explain clustering in incompressible flows. The two most common ones are "preferential concentration" and "multiplicative amplification". Preferential concentration refers to the tendency of heavy particles to avoid vortical regions of the flow. Multiplicative amplification, by contrast, explains clustering in terms of the logarithmic amplification of the sequence of many small kicks that the suspended particles experience.

In order to quantify the relative importance of the two mechanisms it is necessary to compute the fluctuations of the flow-velocity gradients that the particles experience as they move through the flow. We show how this can be achieved systematically by means of perturbation expansions that recursively take into account how the flow affects the actual particle trajectory. We analyse the statistics of particle- and flow-velocity gradients as seen by the particles. Based on these results

we show that in random velocity fields multiplicative amplification has a much stronger effect than preferential concentration, except at very small Stokes numbers. We discuss the implications of these findings for particles suspended in turbulent flows.

Invited Talk DY 34.3 Thu 16:00 HSZ 02
Stochastic population dynamics on rugged fitness landscapes — •Joachim Krug — Institut für Theoretische Physik, Universität zu Köln

Biological evolution is inherently noisy because of random mutations and stochasticity induced by sampling in finite populations. Since the sampling noise is inversely proportional to population size, one expects deterministic dynamics to emerge in large populations, but in practice this regime is hardly every attainable and fluctuations dominate the behavior even in the largest microbial populations. In this talk I will show how the interplay of the stochastic population dynamics with the structure of the underlying fitness landscape can lead to counter-intuitive phenomena such as an adaptive advantage of small populations and a non-monotonic dependence of evolutionary predictability on population size. If time permits, the adaptive benefits of recombination in rugged fitness landscapes will be briefly addressed as well. The talk is based on joint work with Kavita Jain, Johannes Neidhart, Stefan Nowak, Su-Chan Park, Ivan Szendro and Arjan de Visser.

15 min break

Invited Talk DY 34.4 Thu 16:45 HSZ 02
Modeling cancer as a stochastic process — •Tibor Antal — School of Mathematics at Edinburgh University, Edinburgh, UK

Stochasticity is essential when modeling initiation of tumors, progression of tumors from benign to malignant states, or metastasis formation. Many aspects of these phenomena can be modeled by simple multi-type branching processes, and the results compare fairly well with experimental and clinical data. These models then can be used to optimize drug treatments. Spatial heterogeneity of tumors are also important for treatment, and their exploration has recently begun by modeling the interplay between tumor shapes and genetic mutations.

Invited Talk DY 34.5 Thu 17:15 HSZ 02
Von Neumann's growth model: from statistical mechanics to cell metabolism — •Andrea De Martino — Sapienza Universita' di Roma & CNR, Roma, Italy

This talk reviews the basic properties of Von Neumann's model of growth in production economies, mainly from a statistical mechanics perspective. In addition, I will discuss its recent applications in quantitative biology, for the profiling of a cell's metabolic activity and of its thermodynamics. Finally, a class of Boolean constraint-satisfaction problems based on Von Neumann's idea will be presented, whose solutions allow to shed new light on the modular organization of metabolic networks.

DY 35: Reaction-Diffusion Systems

Time: Thursday 15:00–17:30 Location: HÜL 186

DY 35.1 Thu 15:00 HÜL 186
Position and shape control of traveling waves in reaction-diffusion systems — Jakob Löber, •Steffen Martens, and Harald Engel — Technische Universität, Berlin, Deutschland

We present an efficient and easily applicable method to control the position respectively the shape of traveling wave solutions in reaction-diffusion systems according to a desired protocol of movement. Given this protocol, the control function is found as the solution of a perturbatively derived integral equation. In particular, we derived an analytical expression for the space ($\mathbf{r}$) and time (t) dependent control function $f(\mathbf{r}, t)$ that is valid for a large variety of reaction-diffusion systems and many kinds of protocols, e.g., accelerating, decelerating or periodic protocols. Intriguingly, our control method is expressed in terms of the uncontrolled wave profile and its propagation velocity, rendering detailed informations about the reaction kinetics unnecessary. Noteworthy, this method is very close to optimal controls. An extension of the control method allows to control the shape of traveling fronts as well as localized spots in two and three spatial dimensions.

DY 35.2 Thu 15:15 HÜL 186
A continuous transition between two limits of spiral wave dynamics in an excitable medium — •Vladimir Zykov and Eberhard Bodenschatz — Max Planck Institute for Dynamics and Self-Organization, D-37077 Goettingen, Germany

By application of a free-boundary approach we prove the existence of a continuous transition and a full spectrum of solutions between the two known limits of spiral wave dynamics corresponding to trigger-trigger and trigger-phase waves. We identify a control parameter whose essential importance was not realized in earlier studies of spatio-temporal pattern selection in excitable media. The predictions of the free-boundary approach are in good quantitative agreement with results from numerical reaction-diffusion simulations performed on the modified Barkley model.

DY 35.3 Thu 15:30 HÜL 186
Reaction diffusion patterns: Effects of modulations on traveling waves — •Fabian Bergmann, Marius Jakoby, Lisa Rapp, and Walter Zimmermann — Theoretische Physik, 95440 Universität Bayreuth, Germany

In reaction-diffusion models for chemical reactions [1] and biological systems [2] one often finds bifurcations to traveling waves. If such systems in two dimensions are either restricted to narrow stripes [2] or spatially periodic modulated, waves traveling along a preferred direction are found. Results are presented about the dependence of the travel direction of waves on characteristic reaction and diffusion parameters as well as modulation parameters, including the pulling speed of the modulation. In addition a generic description is presented which is valid near the onset of traveling waves. This generic model covers the behavior of modulated traveling waves found in the reaction diffusion systems.

[1] M. Dolnik, A. R. Rovinsky, A. M. Zhabotinsky, I. R. Epstein, Standing Waves in a Two-Dimensional Reaction-Diffusion Model with the Short-Wave Instability, J. Phys. Chem. A 103, 38 (1999)

[2] J. Schweizer, M. Loose, M. Bonny, K. Kruse, I. Mönch, P. Schwille, Geometry sensing by self-organized protein patterns, PNAS 109, 15382 (2012)

DY 35.4 Thu 15:45 HÜL 186
Turing instability in a scalar reaction-diffusion system with delay — •Andreas Otto, Jian Wang, and Günter Radons — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

The existence of diffusion-driven instabilities in scalar systems with time-delay is studied. The so-called Turing instability occurs if the homogeneous steady state of a system is stable in the absence of diffusion but unstable when diffusion is present. As a result spatially inhomogeneous states emerge, which are a subject of current research in physics, biology and chemistry.

To the authors knowledge until now the occurrence of a Turing instability is only known to exist for multi-component systems. In scalar reaction-diffusion systems without or with only one constant delay a Turing instability is not possible. However, diffusion-driven instabilities exist in one component reaction diffusion systems with distributed and/or time-varying delay, which is the topic of this talk.

DY 35.5 Thu 16:00 HÜL 186
Pattern Formation in BZ-AOT Microemulsions Manipulated by Electric Fields — •Patricia Dähmlow and Stefan C. Müller — Otto-von-Guericke University Magdeburg, Germany

Pattern formation in excitable media presents an important phenomenon in biological morphogenesis, electrophysiology and neuronal systems. A rich variety of these patterns can be found in the Belousov-Zhabotinsky (BZ) reaction dissolved in the aerosol OT (AOT) water-in-oil microemulsion (ME).

Using the ferroin- and the bathoferroin-catalyzed BZ reaction, we observed different patterns like Turing patterns, dash waves and discontinuously propagating waves (jumping and bubble waves). By applying an electrical field across the spatially extended solution layer, a

linear drift of these patterns can be observed. Also the layer thickness of the ME plays an important role in the development of the patterns, since a thick layer (220 μm) leads to a "smearing out" of the patterns whereas in a thin layer (100 μm) the drift can be clearly recognized.

The application of an electric field to the microemulsion reveals changes in a number of physical properties of the medium. We follow the assumption that this system can act as a model system for long range interactions beyond local coupling by diffusion processes, thus presenting a concept which could be applicable to long range interactions between neurons.

15 min break

DY 35.6 Thu 16:30 HÜL 186

Influence of polymers on silica gel structure and patterns of Belousov-Zhabotinsky reaction — •Claudia Lenk and J. Michael Köhler — Institut für Chemie und Biotechnik, TU Ilmenau, Germany

Spatio-temporal patterns formed in oscillatory chemical, biological or medical systems resemble the state of the system and their analysis reveals thus information about the underlying processes. Thereby the structure of the media plays an important role for the resulting patterns. To investigate the influence of the structure, we perform experiments of the well-known Belousov-Zhabotinsky (BZ) reaction in a silica gel, where the catalyst Ferroin is immobilized in predefined patterns. To enhance the immobilization different polymers are added to the gel matrix. The influence of the polymers on the gel structure is analyzed by scanning electron microscope and Raman measurements. The best immobilization of Ferroin is observed for gels with polyethylene glycol or poly(styrenesulfonic acid-co-maleic acid) sodium salt. Since, e.g., polyethylene glycol can yield standing wave patterns [1], changes of the oscillatory parameters, like frequency and conduction velocity of the BZ waves, are studied. The relation of these changes to the diffusion properties of the BZ reagents and the chemical and electrical properties of the polymer will be discussed.

[1] D. Cuinas *et al.*, J. Chem. Phys. **128**, 244907 (2008).

DY 35.7 Thu 16:45 HÜL 186

Formation of patchy particles by diffusion limited growth — •Timo Bihr[1,2], Huixin Bao[3], Robin Klupp Taylor[3], Udo Seifert[2], and Ana-Sunčana Smith[1] — [1]Institut für Theoretische Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg — [2]II. Institut für Theoretische Physik, Universität Stuttgart — [3]Institute of Particle Technology, Universität Erlangen-Nürnberg

Patchy particles can be formed by coating polystyrene particles with ascorbic acid as a precursor for gold. The latter precipitates from the solution onto the particle, diffuses on its surface and attaches to a growing gold patch. We investigate the formation of the patch by Monte Carlo simulations and study the effects of gold concentration, binding and unbinding rates, and the diffusion constant. We obtain a variety of dendrite structures which we characterize by their fractal dimension and the power-law characterizing the growth process. The exponents typical for the diffusion limited aggregation are recovered only in the limit of infinite dilution, whereas reaction limited dynamics is obtained at larger densities, depending on the binding affinity. Comparison of modeling with experiments shows that decreasing the concentration of the ascorbic acid results in the decrease of binding affinity, whereas increasing the temperature increases the diffusivity. Consequently in both cases, roughening of the dendrite structure of the patches takes place. The understanding of this process allows us to tune the morphology of the patch on the particle from dense cup-like structures to pure dendrites (H. Bao et al. *Nanoscale*, 2014, DOI: 10.1039/C3NR04016J).

DY 35.8 Thu 17:00 HÜL 186

Studying Protein Assembly with Brownian Dynamics of Patchy Particles: from Microscopic to Macroscopic Rates — •Heinrich Klein[1] and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Germany — [2]BioQuant, Heidelberg University, Germany

Assembly of protein complexes is of high relevance for the functionality of many biological systems like virus shells, the nuclear pore complex or the actin cytoskeleton. Moreover, recent advances in the fabrication of colloidal particles with anisotropic reactivity (*patchy particles*) provide new opportunities to design self-assembling structures. Here we present a novel computational approach for the Brownian dynamics of patchy particles with fully reversible reactions satisfying detailed balance. Different particles stochastically associate and dissociate with microscopic reaction rates depending on their relative spatial positions. We show how macroscopic rates can be inferred from the microscopic rates and the diffusive properties of the assembly intermediates. As an instructive example, we study the assembly of a pentameric ring structure, for which we find excellent agreement between microscopic results and a macroscopic kinetic description without any adjustable parameters. In summary, we have developed a computational framework which accounts for both the diffusional and the reaction processes underlying protein assembly.

DY 35.9 Thu 17:15 HÜL 186

Photoelectrodissolution of n-type silicon: An oscillatory medium with unusual pattern formation — •Konrad Schönleber, Andreas Heinrich, Elmar Miterreiter, Martin Wiegand, Carla Zensen, and Katharina Krischer — Technische Universität München

We investigate the spatial thickness distribution of oxide layers formed at illuminated n-type silicon samples during the anodic electrodissolution in fluoride containing electrolytes by means of spatially resolved ellipsometric imaging. Spontaneous pattern formation in the oxide thickness can be observed for appropriate parameter values while the total current and spatially averaged oxide thickness oscillate simply periodic. The observed patterns typically consist of several regions on the electrode each showing distinct dynamical behavior giving rise to a rich variety of different states, as e.g. so-called 'Chimera states' and other unusual cluster states. In addition, a novel type of spatial organization involving periodically growing and collapsing oscillating domains with peculiar front dynamics are discussed.

DY 36: Brownian Motion and Transport

Time: Thursday 15:00–17:15 Location: ZEU 160

DY 36.1 Thu 15:00 ZEU 160

Statistical mechanics of stochastic ratchets far from equilibrium — •Johannes Blaschke and Jürgen Vollmer — Max-Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Stochastic ratchets (such as the Brownian motor, or the asymmetric adiabatic piston) deliver important insights into the statistical mechanics of non-equilibrium systems.

We examine the motion of an anisotropic particle encountering collisions with a gas far from equilibrium. Contrary to what is observed for a dissipative Maxwell-Boltzmann gas, vanishingly small perturbations to the gas velocity distribution (e.g. via shaking) result in a steady-state drift velocity independent of particle mass in the limit of a massive particle [1].

Inspired by an interesting breakdown of equipartition and linear response theory, here we build on this finding by exploring the statistical mechanics of a gas even further from equilibrium: that of self-propelled swimmers. The kinetic theory shows a rich and surprising behaviour. Furthermore, we show to what extend stochastic thermodynamics and the appropriate fluctuation theorem can account for this behaviour.

[1] J. Blaschke and J. Vollmer, Phys. Rev. E 87, 040201R (2013)

DY 36.2 Thu 15:15 ZEU 160

Resonant Optical Tweezers with Anti-Reflection Coated Titania Microspheres — •Mohammad Kazem Abdosamadi, Anita Jannasch, and Erik Schäffer — Nanomechanics Group, ZMBP - Center for Plant Molecular Biology, University of Tübingen, Auf der Morgenstelle 2, 72076 Tübingen, Germany

Brownian motion is exhibited by an optically tapped particle due to the thermally driven molecules of the surrounding medium. This motion is often considered to be a frequency-independent phenomenon which is known as a white noise process. However, fluid entrainment influences the particle in the trap and results in a frequency-dependent motion. Therefore, the power spectral density (PSD) of the noise that drives the motion is "colored". The "colored noise" of the Brownian motion can change the behavior of an optical trap from an overdamped oscillator to a resonant one. Here, our goal was to amplify this resonance. Theoretical calculations predict that particles with a large diameter and a high trap stiffness enhance the resonance effect. Therefore, we synthesized large anti-reflection coated titania microspheres. These microspheres have a high trap stiffness in the optical trap. In comparison to our previous work [Jannasch, Phys. Rev. Lett. 2011], the results showed a roughly 4 times enhancement of the resonance in acetone. The resonant behavior could be used as a sensor in analogy to other resonant probes such as an atomic force microscope cantilever.

DY 36.3 Thu 15:30 ZEU 160

Hydrodynamically enforced entropic trapping of Brownian particles — •Steffen Martens[1], Gerhard Schmid[2], Arthur Straube[3], Lutz Schimansky-Geier[3], and Peter Hänggi[2] — [1]Technische Universität, Berlin, Deutschland — [2]Universität Augsburg, Augsburg, Deutschland — [3]Humboldt-Universität zu Berlin, Berlin, Deutschland

In small systems spatial confinement causes entropic forces that in turn implies spectacular consequences for the control for mass and charge transport. In view of its importance, recent efforts in theory triggered activities which allow for an approximate description that involves a reduction of dimensionality; thus making detailed predictions tractable. Up to present days, the focus was on the role of conservative forces and its interplay with confinement. Within the presented work, we overcome this limitation and succeeded in considering also "magnetic field" like, so termed non-conservative forces that derive from a vector potential [S. Martens et al., *Phys. Rev. Lett.* **110**, 010601 (2013)]. A relevant application is the fluid flow across microfluidic structures where a solute of Brownian particles is subject to both, an external bias and a pressure-driven flow. Then a new phenomenon emerges; namely, the intriguing finding of identically vanishing average particle flow which is accompanied by a colossal suppression of diffusion. This entropy-induced phenomenon, which we termed *hydrodynamically enforced entropic trapping*, offers the unique opportunity to separate particles of the same size in a tunable manner [S. Martens et al.,*Eur. Phys. J. ST* **222**, 2453-2463 (2013)].

DY 36.4 Thu 15:45 ZEU 160

Computersimulation of colloidal particles in channel geometries — •Ullrich Siems and Peter Nielaba — University of Konstanz

This talk presents the results of Brownian Dynamics Simulation of paramagnetic particles confined to two-dimensional micro-channels under the influence of external forces. Two-dimensional colloidal dispersions are well known model systems for a variety of problems on different length scales and have also some applications to microfluidic devices. Confinement into channels can have a great influence on diffusion and transport properties in such systems. A good agreement of Brownian Dynamic Simulation with experiments has been found in the past.

DY 36.5 Thu 16:00 ZEU 160

Calculation of the waiting time distribution with a Fokker Planck equation: hopping in a one-dimensional periodic potential — •Robert Gernert[1], Clive Emary[2], and Sabine H.L. Klapp[1] — [1]Institut für theoretische Physik, Technische Universität Berlin — [2]Department of Physics and Mathematics, University of Hull, United Kingdom

"How long will a complex stochastic process take?" The waiting time distribution (WTD) gives us the answer. The question is important in Brownian as well as in quantum transport [1,2], because it allows to identify the, possibly several, relevant time scales of non-equilibrium motion and to get these single-particle resolved.

Recent developments in quantum transport[2] have shown that the WTD is (especially for short times) more detailed than full counting statistics, i.e. than the cumulants of motion like mean position, mean squared displacement or non-Gaussian parameter.

A way to calculate the WTD directly with a Fokker-Planck equation is presented. As an example the one-dimensional overdamped motion of one Brownian particle in a washboard potential is investigated.

We also present a Master equation approach, based on [3], which gives analytic access to the WTD. Both approaches are verified by comparison to Brownian dynamics simulations.

[1] R.D.L. Hanes, C. Dalle-Ferrier, M. Schmiedeberg, M.C. Jenkins, S.U. Egelhaaf, Soft Matter 8, 2714 (2012)
[2] M. Albert, C. Flindt, M. Büttiker, PRL 107, 086805 (2011)
[3] C. Emary, R. Gernert, S.H.L. Klapp, PRE 86, 061153 (2012)

15 min break

DY 36.6 Thu 16:30 ZEU 160

Convex Hulls of Random Walks: Large-Deviation Properties — •Gunnar Claussen[1], Satya N. Majumdar[2], and Alexander K. Hartmann[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Laboratoire de Physique Théorique et Modèles Statistiques, Université Paris-Sud

We numerically consider two-dimensional time-discrete random walks of length T represented through sets $\{\vec{\delta}_i\}$ of vectors denoting the steps $i \leq T$. Motivated by modeling animal home ranges [1], we are interested in area A and perimeter L of the convex hull over the trajectory $\vec{x}(t)$ of this walk. As previous studies determined the analytical averages $\langle A\rangle$ and $\langle L\rangle$ [2], we aim at the according distributions $P(A)$ and $P(L)$ by application of a Monte Carlo method [3] which allows us to sample within ranges of particularly rare values of A and L, leading to probabilities such as 10^{-300}. The resulting distributions can be compared with respect to their scaling behaviour, their rate functions $\Phi(s) = -T^{-1} \cdot \log P(s)$ (with $s = A/A_{\max}$ or $s = L/L_{\max}$, respectively) and standard analytical distribution functions $p(A)$ and $p(L)$ like the Gumbel distribution. Our analyses of these properties resulted in the obtaining of asymptotic values for the corresponding parameters and exponents for $T \to \infty$. A multitude of walk lengths T, open and closed walks and various types of step displacements $\vec{\delta}_i$ have been covered by our simulations.

[1] L. Giuggioli et al., PLoS Comput. Biol. 7 (2011) e1002008
[2] S.N. Majumdar et al., J. Stat. Phys. 138 (2010) 995-1009
[3] A.K. Hartmann, Eur. Phys. J. B 84 (2011) 627-634

DY 36.7 Thu 16:45 ZEU 160

Multi-terminal Thermoelectric Transport in a Magnetic

Field: Bounds on Onsager Coefficients and Efficiency — •Kay Brandner[1], Julian Stark[1], Keiji Saito[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart — [2]Department of Physics, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Japan 223-8522

Thermoelectric transport in non-interacting systems involving an arbitrary number of terminals is discussed in the presence of a magnetic field breaking time-reversal symmetry. We derive a universal bound on the Onsager coefficients that depends only on the number of terminals [1,2]. This bound implies bounds on the efficiency and on efficiency at maximum power for heat engines and refrigerators. To illustrate our results, we introduce a simple classical model using four terminals for a thermoelectric engine based on the Nernst effect [3]. Within this setup, the predicted bound on the efficiency can indeed be saturated for large magnetic fields and small fugacity in the thermochemical reservoirs.

[1] K. Brandner, K. Saito and U. Seifert, Phys. Rev. Lett. **110** 070603 (2013)
[2] K. Brandner and U. Seifert, New J. Phys. **15** 105003 (2013)
[3] J. Stark, K. Brandner, K. Saito and U. Seifert, arXiv:1310.1195v1 (2013)

DY 36.8 Thu 17:00 ZEU 160

Advanced data analysis by the distribution of diffusivities — •Michael Bauer and Günter Radons — Technische Universität Chemnitz, Germany

Single-particle tracking (SPT) provides a useful approach to observe individual tracers and characterize transport processes in physical and biological systems. However, an analysis based on well-established quantities, such as mean squared displacements (msd), often obscures the interesting properties of complex systems. To improve the interpretation of SPT experiments we introduced the distribution of diffusivities. We demonstrated its applicability to heterogeneous diffusion in a two-layer system and showed its relation to ensemble-based methods such as pulsed field gradient nuclear magnetic resonance (PFG NMR) [1]. Furthermore, we analyzed processes with direction-dependent diffusion coefficients [2], which are of great interest for anisotropic diffusion, e.g., of elongated molecules or in porous media. Additionally, our new method was extended to the distribution of generalized diffusivities to characterize data from anomalous diffusion processes [3]. In our contribution we will explain the properties and features of the distribution of diffusivities. We apply our method to different systems and show the advantages over conventional analysis methods.

[1] M. Bauer et al., J. Chem. Phys. 135, 144118 (2011)
[2] M. Heidernätsch et al., J. Chem. Phys. 139, 184105 (2013)
[3] T. Albers and G. Radons, EPL 102, 40006 (2013)

DY 37: Fluid Dynamics and Turbulence

Time: Thursday 15:00–16:30 Location: ZEU 146

DY 37.1 Thu 15:00 ZEU 146

Dynamic emptying and dynamic wetting transitions in dragged meniscus problems — •Uwe Thiele[1,2], Mariano Galvagno[1], Hender Lopez[3], and Dmitri Tseluiko[1] — [1]Department of Mathematical Sciences, Loughborough University, UK — [2]Institut für Theoretische Physik, Universität Münster, Germany — [3]School of Physics, University College Dublin, Ireland

We study the transfer of a non-volatile liquid from a bath onto a flat plate that is drawn out of the bath. After reviewing previous works [1,2] we use a long-wave mesoscopic hydrodynamic model that incorporates wettability via a Derjaguin (disjoining) pressure to analyse steady meniscus profiles as the plate velocity is changed. We identify four qualitatively different dynamic transitions between microscopic and macroscopic coatings that are out-of-equilibrium equivalents of equilibrium unbinding transitions, namely, continuous and discontinuous dynamic emptying transitions and discontinuous and continuous dynamic wetting transitions [3]. We discuss several features that have no equivalent at equilibrium, e.g., we show that the change from the continuous to the discontinuous dynamic emptying transition involves the emergence of exponential snaking caused by the existence of infinitely many heteroclinic orbits close to a heteroclinic chain in an appropriate 3d phase space [4].

[1] A. O. Parry et al., Phys. Rev. Lett. 108:246101, 2012; [2] J. Ziegler, J. H. Snoeijer, J. Eggers. Eur. Phys. J.-Spec. Top. 166:177-180, 2009; [3] M. Galvagno et al., arxiv.org/abs/1311.6994; [4] M. Galvagno, D. Tseluiko, U. Thiele, arxiv.org/abs/1307.4618

DY 37.2 Thu 15:15 ZEU 146

Stokes flow in complex domains — •Andreas Lemmer and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, D-70569 Stuttgart

Numerically solving the Stokes equation in complex domains like porous media is computationally difficult because of the large number of unknowns, the complicated domain geometry and the velocity-pressure coupling. We present a domain decomposition method on a uniform, staggered grid which is completely parallelized using only non-blocking communication, therefore achieving high parallel efficiency[1]. This method is used to numerically solve the Stokes equation on a synthetic sample of a laboratory sized Fontainebleau sandstone. The cubic sample with side length $15mm$ is discretized with resolutions from $117\mu m$ down to $458nm$, resulting in sample sizes from 128^3 to 32768^3 grid cells[2]. The flow calculation on the sample with 2048^3 grid cells and over $5 \cdot 10^9$ unknowns on the bwGrid Cluster, HLRS Stuttgart on 512 processors took 30 hours.

[1] A. Lemmer, R. Hilfer, to be published
[2] R. Hilfer, T. Zauner: High-precision synthetic computed tomography of reconstructed porous media, Phys.Rev.E, 84, 062301 (2011)

DY 37.3 Thu 15:30 ZEU 146

Evolution equations for two dimensional elliptic shaped gaussian vortices — •Markus Blank-Burian — Institut für Physikalische Chemie, WWU Münster, Deutschland

The easiest model to describe two dimensional vortices in turbulent flows is the point vortex model. This model has an inherent problem, as it can not describe either attraction or repulsion of two vortices. By studying numerical and experimental data, one can see, that in first approximation two interacting vortices maintain a nearly elliptic gaussian shape for a rather long time. Vortices with the same sign attract each other and orientate themselves parallel with an angle of approximately 45° to their connecting vector. Vortices with different sign orient themselves nearly perpendicular to each other while moving in the same direction.

Based on an idea in [1], one can derive equations of motion for two interacting elliptically shaped gaussian vortices, describing their evolution in time. This model then correctly predicts attraction and repulsion of two vortices, depending on the strenth and orientation of the vortices. The characteristic angles of 45° are found stable as well. The famous Lamb-Oseen vortex is contained as a limiting case of symmetric shape.

[1] Friedrich, Friedrich: Generalized vortex-model for the inverse cascade of two-dimensional turbulence, http://arxiv.org/abs/1111.5808

DY 37.4 Thu 15:45 ZEU 146

The solar wind as a turbulence laboratory- some new quantitative points of contact between theory and solar wind observations — •Sandra Chapman[1,2,3], Khurom Kiyani[4,1], Kareem Osman[1], Bogdan Hnat[1], and Ersilia Leonardis[1] — [1]CFSA, Physics, University of Warwick, UK — [2]MPIPKS, Dresden, Germany — [3]Mathematics and Statistics, UIT, Norway — [4]Laboratoire de Physique des Plasmas, Ecole Polytechnique, Saclay, France

The solar wind flow has a Reynolds number of order 10ˆ5. Single point sattelite observations of plasma parameters suitable for the study of turbulence are on timescales from below ion kinetic scales up to days. We will present methodology to quantify the scaling properties of turbulence from in-situ satellite observations in the solar wind that address the problems of scaling over a finite range and restricted sampling of rare extreme events.

Ideal fluid turbulence is characterized by non-Gaussian distributions of fluctuations which become progressively fat-tailed on smaller scales, and which exhibit a multifractal scale invariance, a behaviour also seen in the MHD inertial range of turbulence in the solar wind. We show that below the ion kinetic scales there is instead a cross-over to a quan-

titatively distinct global scale invariance and discuss the implications for the physics of kinetic range turbulence. Solar wind plasma turbulence is anisotropic due to the presence of a background field. We will discuss how this anisotropy also orders the scaling properties seen in solar wind turbulence.

DY 37.5 Thu 16:00 ZEU 146

Generation of turbulence with an active grid — •Lars Kröger, Nico Reinke, Gerd Gülker, and Joachim Peinke — ForWind, Center for Wind Energy Research, University of Oldenburg, D-26129 Oldenburg, Germany

Turbulent fluid flows are omnipresent in our everyday life. Especially turbulence in the atmospheric boundary layer is a very important topic for wind energy research. As experiments in nature are somewhat limited and could mostly not take place under reproducible circumstances, wind tunnel measurements are necessary. Placing grids behind the wind tunnel nozzle is a common way to generate turbulence in a laboratory experiment. So called active grid consisting of horizontal and vertical oscillating rods with flaps are used in some investigations providing an improved option to generate dynamically driven turbulence with a wide range of statistical behaviour. Reproducible and statistical well defined turbulence could be generated with defined excitation protocols of the active grid flaps. In our experiments, we are using active grids in two wind tunnels with different dimensions. In this presentation hotwire and PIV measurements of the grid wakes are presented in order to investigate the scaling ability of the turbulent flow. For this, the decaying turbulence of different excitation protocols of the two mentioned grids is characterized by measurements of the velocity, the power spectra and turbulence intensity.

DY 37.6 Thu 16:15 ZEU 146

Hierarchy of structure function relations for locally isotropic MHD turbulence — •Jan Friedrich[1], Holger Homann[2], Tobias Schäfer[3], and Rainer Grauer[1] — [1]Theoretische Physik I, Ruhr-Universität, 44780 Bochum, Germany — [2]Laboratoire J.-L. Lagrange, Universite de Nice-Sophia Antipolis, CNRS, France — [3]Department of Mathematics, College of Staten Island, CUNY, USA

We investigate the structure of locally isotropic magneto-hydrodynamic (MHD) turbulence by means of exact equations for magnetic and velocity structure functions. To this end we make use of the calculus of isotropic tensors for MHD turbulence introduced by Chandrasekhar [1]. A hierarchy of structure function equations is obtained, beginning with the MHD analagon of Kolmogorov's four-fifths law of hydrodynamics. The influence of the mean-magnetic field is discussed within the context of the Iroshnikov-Kraichnan phenomenology [2], [3]. The next order equation relates the third- and fourth-order structure functions and is the first order which provides a direct dependence between the longitudinal and the transverse structure functions based on the dynamics. At this order, we have to deal for the first time with pressure contributions. The influence of the additional magnetic pressure is discussed in comparison to the hydrodynamic case and the obtained relations are checked by direct numerical simulations of three-dimensional MHD turbulence.

[1] S. Chandrasekhar, Proc. R. Soc. Lond. A, 204, 1079 (1951)
[2] P.S. Iroshnikov, Sov. Astron. 7, 566-71 (1964)
[3] R.H. Kraichnan, Phys. Fluids 8, 1385-7 (1965)

DY 38: Glasses and Glass Transition - Part II (joint session CPP/ DY/DF)

Time: Thursday 15:00–17:30 Location: ZEU 114

Invited Talk DY 38.1 Thu 15:00 ZEU 114

Microscopic investigation of creep in glasses — Tatjana Sentjabrskaja[1], Pinaki Chaudhuri[2], Wilson Poon[3], Jürgen Horbach[2], Stefan Egelhaaf[1], and •Marco Laurati[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Theoretische Physik II, Heinrich Heine University, Düsseldorf, Germany — [3]SUPA and COSMIC, The University of Edinburgh, United Kingdom

The microscopic origin of the creep rheological response of colloidal glasses is investigated, based on the particle-level dynamics measured by confocal microscopy during application of a step stress. Sub-diffusive single-particle dynamics are the microscopic signature of creep. At a more local scale enhanced dynamic activity is observed at random locations, with the number of active regions following the time-dependence of the macroscopic strain. Instead, diffusive dynamics characterise the flowing system, with a transient super-diffusive regime during the onset of flow. Transient super-diffusion coincides with the appearance of enhanced dynamics in a specific region of the system, which subsequently rapidly expands and finally spans the whole system when the steady state of flow is reached.

Invited Talk DY 38.2 Thu 15:30 ZEU 114

Getting into shape: Jamming of frictional particles. — •Matthias Schröter, Jean-François Métayer, Frank Rietz, and Max Neudecker — MPI for Dynamics and Self-Organization

In recent years the Jamming paradigm has been promoted as a grand unifying theory of particulate soft matter systems like foams, colloids, emulsions, and granular media [1,2]. However, this approach has mostly evolved from simulations of soft, perfect spheres. Real world particulate systems are often "rough" on either a microscopic or a particle scale. In the first case we talk about friction, in the second about non-spherical shapes.

This talk will use 3D imaging techniques such as X-ray tomography to provide insight into the mechanical stability of tetrahedra packings [3], the volume response of sheared granular media, and the first order phase transition occurring at Random Close Packing. We will show that in non of these three examples the underlying physics is adequately described by the Jamming paradigm.

[1] A. Liu and S. Nagel, Ann. Rev. Cond. Mat. Phys. **1**, 347-369 (2010)
[2] M. van Hecke, J. Phys.: Condens. Matter **22**, 033101 (2010)
[3] M. Neudecker, S. Ulrich, S. Herminghaus, and M. Schröter, Phys. Rev. Lett. **111**, 028001 (2013)

DY 38.3 Thu 16:00 ZEU 114

Glassy Dynamics of Collapsed Isolated Polymer Chains — •Martin Tress[1], Emmanuel Urandu Mapesa[1], Manfred Reiche[2], and Friedrich Kremer[1] — [1]Universität Leipzig — [2]MPI für Mikrostrukturphysik, Halle

While structure and conformation of condensed, isolated low molecular weight and polymeric molecules are well explored, knowledge concerning their dynamics, as measured in a broad spectral range and at widely varying temperatures is sparse. To overcome this, Broadband Dielectric Spectroscopy is combined with nano-structured electrodes having 35 nm separation and the dynamics of collopsed isolated poly(2-vinylpyridine) (P2VP) globules is measured. The collapsed globule conformation is revealed by Atomic Force Microscopy scans of the identical samples with an average globule volume corresponding to the estimate for a single chain (using the molecular weight and bulk density). Hence, for the first time the dynamic glass transition of condensed isolated polymer chains is directly measured and found to be bulk-like; only segments close (< 0.5 nm) to the substrate are weakly slowed down. The observation of bulk-like dynamics is in full accord with the length scale on which the dynamic glass transition is to be expected. In contrast, the emersion of new, slower relaxation modes is attributed to attractive interactions of the P2VP segments with the supporting silica surface, a finding which is corroborated by complementary infrared experiments. Our approach paves the way for numerous experiments on the dynamics of isolated molecules.

15 min break

DY 38.4 Thu 16:30 ZEU 114

A direct quantitative measure of surface mobility in a glassy polymer — Yu Chai[1], •Thomas Salez[2], Joshua D. McGraw[3], Michael Benzaquen[2], Kari Dalnoki-Veress[4], Elie Raphaël[2], and James A. Forrest[1] — [1]University of Waterloo, Canada — [2]ESPCI, Paris, France — [3]Saarland University, Saarbrücken, Germany — [4]McMaster University, Hamilton, Canada

The simple geometry of a polymer film on a substrate with a step at the free surface is unfavourable due to the excess interface induced by the step, thus allowing for a new nanoprobe of the melt state rheology.

After recalling the experimental technique, we demonstrate how the same theoretical tools enable to understand the surface evolution of thin polymer films below the glass transition temperature T_g. While above T_g the entire volume between the substrate and the free surface participates to the flow, below T_g only a near surface region responds to the excess interfacial energy. In the latter case, the developed thin film theory for flow limited to the free surface region is in excellent agreement with experimental data. Strikingly, the system transitions from whole film flow to surface localized flow over a narrow temperature region near the bulk glass transition temperature. The measurements and model presented provide a quantitative measure of the surface mobility in a sample geometry where the confinement of polymer chains and substrate effects are negligible. Therefore, this study may help to solve further the ongoing controversy around glass transition in polymer films.

DY 38.5 Thu 16:45 ZEU 114

Effects of soft confinement on the glass dynamics of glycerol, studied by deuteron NMR — •Michael Lannert[1], Markus Rosenstihl[1], Thomas Blochowicz[2], Bernd Stühn[2], and Michael Vogel[1] — [1]Institut für Festkörperphysik, Hochschulstraße 6, 64289 TU Darmstadt — [2]Institut für Festkörperphysik, Hochschulstraße 8, 64289 TU Darmstadt

The dynamics of glycerol in a microemulsion with droplet diameters ranging from 2nm to 9nm were investigated by deuteron NMR in the temperature range 150K - 330K. While previous studies of liquid dynamics in confinement mostly used solid matrices, microemulsion droplets formed by AOT surfactants and toluol/m-xylol provide a soft confinement. Deuteron NMR longitudinal (T_1) and transversal (T_2) spin relaxation times, solid echo spectra, and two time correlation functions were recorded. High temperature dynamics are independent from droplet diameter and a Vogel-Fulcher-Tamann temperature dependence was observed. The line shape transition occurs at 240K for all studied droplet sizes, but is broader in confinement than in bulk, indicating a broadening of the distribution of correlation times. Time constants obtained from the measured correlation functions exhibit a weaker, Arrhenius temperature dependence. Detailed analysis suggests that the reorientation results from the rotational diffusion of whole droplets rather than individual molecules.

DY 38.6 Thu 17:00 ZEU 114

Single molecule diffusion measurements in highly viscous media — •Dominik Wöll[1,2] and Maren Dill[2] — [1]Zukunftskolleg, Universität Konstanz, D-78457 Konstanz — [2]Fachbereich Chemie, Universität Konstanz, D-78457 Konstanz

Single molecule diffusion measurements in highly viscous media require a method which can readily detect very low diffusion coefficients. Single molecule fluorescence tracking typically becomes rather unreliable for diffusion coefficients below 10^{-18} m^2 s^{-1} due to the limited accuracy in determining single molecule positions of a few nanometres and the need for a very high stability of the optical system, even for long-time measurements of several hours. We developed a photocleavable energy transfer dyad which, so far, has allowed us to extend the range of single molecule (pair) diffusion measurements by three orders of magnitude and to determine slow single molecule motion in polymer films in close vicinity to their glass transition temperature. As a FRET pair, we used a perylene and a terrylene diimide derivative, two very efficient and stable fluorophores ideal for single molecule fluorescence spectroscopy. A phenacyl derivative was chosen as the photolabile moiety which could be cleaved with UV light. Initially, the two fluorophores are covalently bound to each other and move correlated before they are cleaved by a UV light pulse and their diffusive separation gives access to low diffusion coefficients of down to 10^{-21} m^2 s^{-1} and beyond.

DY 38.7 Thu 17:15 ZEU 114

Intermittent Quakes on Surface of Soft Glassy Suspensions — •Tadashi Kajiya[1], Tetsuharu Narita[2], Velonique Schmitt[3], Francois Lequeux[2], and Laurence Talini[2] — [1]Max Plank Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany — [2]PPMD-SIMM, UMR 7615 CNRS, UPMC, ESPCIParisTech, 10 rue Vauquelin, 75231 Paris Cedex 05, France — [3]CRPP, UPR 8641 CNRS, Universite Bordeaux 1, 115 Avenue Schweitzer, 33600 Pessac, France

We present measurements of the thermal fluctuations of the free surface of oil-in-water emulsions which exhibit a glassy behavior. The Surface Fluctuation Specular Reflection (SFSR) technique was applied to measure the free surface fluctuation. SFSR technique permits to probe the height of the fluctuations of liquid surface using the reflection of a laser beam projected on the target surface [1].

We found that when the volume fraction of the oil droplets is close to or larger than the disordered packing volume fraction, the free surface exhibits abnormal fluctuations, consisting of rare but large amplitude quakes. From a statistical analysis of the fluctuation signal, we also found that such large fluctuations become more prominent as the system ages. These quakes correspond to large changes in the local slope of the free surface over a few tenths of a second. We conjecture that such quakes reflect the dynamics peculiar to glassy systems driven by the relaxations of internal stress [2].

[1] A. Tay et al. Rev. Sci. Instrum. 79, 103107 (2008) [2] T. Kajiya et al. Soft Matter. 9, 11129 (2013).

DY 39: Graphene: Spintronics, Transistors, and Sensors (joint session HL/DY/DS/MA/O/TT)

Time: Thursday 15:00–18:00 Location: POT 081

DY 39.1 Thu 15:00 POT 081

Graphene's RF Potential: How harmful is the Zero Bandgap? — Kyle D. Holland[1], Navid Paydavosi[1], Neophytos Neophytou[2], •Diego Kienle[3], and Mani Vaidyanathan[1] — [1]Department of Electical and Computer Engineering, University of Alberta — [2]Institute for Microelectronics, Technical University of Vienna — [3]Institute of Theoretical Physics I, University of Bayreuth

With the aid of self-consistent quantum-mechanical simulations and simple expressions for the radio-frequency (RF) metrics, we examine the impact of a lack of a bandgap on limiting the RF potential of graphene transistors. Considering various RF figures of merit, we show that the lack of a bandgap leads to all RF metrics being optimal when the bias point is chosen such that the drain Fermi level aligns with the Dirac point at the midpoint of the channel. We further quantify the precise extent to which the lack of a bandgap limits the transistor's cutoff frequencies, an issue that has been flagged as requiring crucial attention to make graphene transistors competitive. For an 18-nm channel length, we show that the extrinsic unity-current-gain frequency could be improved by 300 GHz and the unity-power-gain frequency could be doubled if a bandgap could be introduced to reduce the output conductance to zero. [1] K. D. Holland, N. Paydavosi, N. Neophytou, D. Kienle, and M. Vaidyanathan, IEEE Trans. Nanotechnol. 12, 566 (2013).

DY 39.2 Thu 15:15 POT 081

Atomic layer deposited aluminum oxide on epitaxial graphene without surface activation — •Peter Wehrfritz[1], Florian Speck[2], Felix Fromm[1], Stefan Malzer[3], and Thomas Seyller[1] — [1]TU Chemnitz, Institut für Physik, Chemnitz, Deutschland — [2]FAU Erlangen-Nürnberg, Department Physik, Erlangen, Deutschland — [3]FAU Erlangen-Nürnberg, Angewandte Physik, Erlangen, Deutschland

Graphene with its high charge carrier mobility is a promising material for analog RF field effect transistors. The preparation of the required insulating layer is still challenging. Atomic layer deposition (ALD) has been extensively studied in the context of alternative dielectrics for silicon-based field effect transistors owing to its capabilities to produce high-quality, homogeneous oxide layers. However, nucleation of ALD growth is strongly suppressed on inert graphene surfaces.

In this contribution we present an approach to obtain conformal aluminum oxide (Al_2O_3) on epitaxial monolayer graphene on silicon carbide (SiC). We demonstrate that closed layers of Al_2O_3 can be deposited on the so called buffer layer. This buffer layer covered by ALD-Al_2O_3 can then be decoupled from the SiC substrate by means of hydrogen intercalation yielding quasi-freestanding monolayer graphene with an insulating dielectric on top. We investigated the quality of the graphene layer and ALD-Al_2O_3 using X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, AFM, and Hall effect measurements.

DY 39.3 Thu 15:30 POT 081

Spin-dependent negative differential resistance in composite graphene superlattices — •Christopher Gaul[1,2], Javier Munárriz[2], Andrey V Malyshev[2], Pedro A Orellana[3], Cord A Müller[4], and Francisco Domínguez-Adame[2] — [1]Max-Planck-Institut für Physik Komplexer Systeme, Dresden — [2]Universidad Complutense de Madrid, Spain — [3]Universidad Técnica Federico Santa María, Casilla 110 V, Valparaíso, Chile — [4]Fachbereich Physik, Universität Konstanz

We propose and study a compound system of a graphene nanoribbon and a set of ferromagnetic insulator strips deposited on top of it. The periodic array of ferromagnetic strips induces a proximity exchange splitting of the electronic states in graphene, resulting in the appearance of a superlattice with a spin-dependent energy spectrum. We find clear signatures of spin-dependent negative differential resistance. The electric current through the device can be highly polarized and both the current and its polarization manifest non-monotonic dependence on the bias voltage. The device operates therefore as an Esaki spin diode, which opens possibilities to design new spintronic circuits.

Phys. Rev. B 88, 155423 (2013)

DY 39.4 Thu 15:45 POT 081

Exchange coupling between localized defect states in graphene nanoflakes — •Matthias Droth and Guido Burkard — University of Konstanz, Germany

Graphene nanoflakes are interesting because electrons are naturally confined in these quasi zero-dimensional structures, thus eluding the need for a bandgap. Defects inside the graphene lattice lead to localized states and the spins of two such localized states may be used for spintronics. We perform a tight-binding description on the entire system and, by virtue of a Schrieffer-Wolff-transformation on the bonding and antibonding states, we extract the coupling strength between the localized states. The coupling strength allows us to estimate the exchange coupling, which governs the dynamics of singlet-triplet spintronics.

DY 39.5 Thu 16:00 POT 081

Novel fabrication method of lateral spin valve devices based on graphene on hexagonal boron nitride — Marc Drögeler[1], Frank Volmer[1], •Maik Wolter[1], Bernat Terrés[1], Kenji Watanabe[3], Takashi Taniguchi[3], Gernot Güntherodt[1], Christoph Stampfer[1,2], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany, EU — [2]Peter Grünberg Institute (PGI-8/9), Forschungszentrum Jülich, 52425 Jülich, Germany, EU — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

Despite tremendous efforts in improving graphene-based spin transport devices the measured spin lifetimes are still orders of magnitude less than theoretically predicted. Contact-induced spin dephasing has recently been identified as the bottleneck for spin transport through Co/MgO spin injection and detection electrodes. It can, however, significantly be suppressed for devices with large contact resistance area products [1]. Simultaneously, a strong reduction of the charge carrier mobility is usually observed. We present a new method to fabricate graphene-based non-local spin valves on hexagonal boron nitride yielding spin lifetimes above 3 ns, spin diffusion length above 10 μm and large charge carrier mobilities above 30.000 cm^2/Vs.

[1] F. Volmer *et al.*, Phys. Rev. B **88**, 161405(R) (2013).

This work has been supported by DFG through FOR 912 and by EU through Graphene Flagship.

DY 39.6 Thu 16:15 POT 081

Suppression of contact-induced spin dephasing in graphene/Co/MgO$_x$ spin-valve devices by successive oxygen treatments — Frank Volmer, •Christopher Franzen, Marc Drögeler, Eva Maynicke, Nils von den Driesch, Maren Laura Boschen, Gernot Güntherodt, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany

By successive oxygen treatments of graphene non-local spin-valve devices we achieve a gradual increase of the contact resistance area products R_cA of the Co/MgO$_x$ spin injection and detection electrodes and a transition from linear to non-linear characteristics in the corresponding dV/dI-curves. With this manipulation of the contacts both spin lifetime and amplitude of the spin signal can significantly be increased by a factor of seven in the same device. This demonstrates that contact-induced spin dephasing is the bottleneck for spin transport in graphene devices with small R_cA values [1]. With increasing R_cA we furthermore observe the appearance of a second charge neutrality point (CNP) in gate dependent resistance measurements. Simultaneously we observe a decrease of the gate voltage separation between the two CNPs. The strong enhancement of the spin transport properties as well as the charge transport will be explained by the same gradual suppression of a Co/graphene interaction by improving the oxide barrier.

Work was supported by DFG/FOR 912 and EU/Graphene Flagship.

[1] F. Volmer *et al.* Phys. Rev. B **88**, 161405 (2013).

Coffee break (15 min.)

DY 39.7 Thu 16:45 POT 081

Development of an amperometric H2O2 sensor based on graphene — •Masoumeh Sisakhti[1], Alexander Zöpfl[2], Jonathan Eroms[1], Thomas Hirsch[2], and Christoph Strunk[1] — [1]Institut für Experimentelle und Angewandte Physik,Universität Regensburg — [2]Institut für analytische Chemie,Universität Regensburg

The precise detection of Hydrogen peroxide (H2O2) has been a widely researched topic and the focus of a vast amount of attention, owing to its vital role in biological systems, as well as its utility in food, pharmaceutical and biochemical industries.

The objective of this work is to investigate a novel nonenzymatic, amperometric sensor for reliable determination of H2O2 based on graphene.

We produced graphene sensors based on three types of graphene: exfoliated graphene, CVD grown graphene and reduced graphene oxide and carried out cyclic voltammetry and amperometric experiments using a CH Instrument electrochemical analyzer. We demonstrate that all three graphene materials show excellent sensitivity to the catalytic reduction of H2O2 and are able to detect H2O2 concentrations down to 0.1 mM. rGO as well as graphene prepared by CVD are promising candidates for sensor applications since they are able to detect hydrogen peroxide with high sensitivity at moderate electrode potentials. Both materials are superior in the signal-to-noise ratio compared to exfoliated graphene. A further conjugation of enzymes to the defects within the carbon nano material as well as the assembly of 2D-layered composite materials will be perspective to biosensor applications.

DY 39.8 Thu 17:00 POT 081

Controlled chemical modification of graphene for applications in biosensing — •Marco R. Bobinger, Max Seifert, Anna Cattani-Scholz, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Given its exceptional chemical and mechanical stability as well as its unique electronic properties, graphene is an extremely promising platform for biosensors. In order to use graphene in the biological environment and to improve sensing specificity and device performance, chemical functionalization schemes are needed to allow stable grafting of organic and bioorganic molecules onto graphene. In particular for applications in bioelectronics, the influence of the chemical functionalization of graphene on the generation of defects, strain, and doping has to be balanced with the desired modulation of the electronic properties of the produced graphene-organic hybrid material. In this work the effect of the controlled chemical modification of large area CVD-grown graphene via ozone treatment is investigated. This process creates sp3-like defects, related to covalently bound surface groups, e.g. OH-. Such ozone-treated surfaces are characterized by Raman- and X-ray photoelectron spectroscopy in order to investigate the degree of surface modification and the chemical composition of the surface terminations. The generated anchor groups are further used as binding sites for the modification of graphene with organic molecules.

DY 39.9 Thu 17:15 POT 081

Functionalization of Graphene for Bioelectronic Applications — •Alina Lyuleeva[1], Lucas Hess[1], Frank Deubel[2], and Jose Antonio Garrido[1] — [1]Walter Schottky Institut, TU München, 85748 Garching — [2]Wacker Chemie AG, 81379 München, Germany

With its fascinating structural, chemical and electronic properties, graphene outperforms many materials and is expected to pare the way for a vast range of applications such as transparent electrodes, energy storage devices, high-frequency electronics, or biosensors. The performance of the devices for these various applications can be enhanced with the help of surface functionalization, allowing a versatile modification of the properties of this material. Here, we report on

the covalent and thus robust functionalization of CVD graphene with enzymes for the development of novel devices for bioelectronic applications. Graphene solution-gated field-effect transistors (SGFETs) are functionalized using a controlled grafting of polymethacrylate (PMA) brushes. We will show how this material platform can be used for further functionalization with the enzyme acetylcholinesterase (AChE). The enzymes' activity can be monitored with the modified-graphene transistor allowing both the measurement of the concentration of the neurotransmitter acetylcholine as well as the inhibition of the enzyme by neurotoxins such as nerve agents or pesticides. Our study demonstrates the potential of graphene-based functionalized transistors for biosensing and bioelectronic application.

DY 39.10 Thu 17:30 POT 081

Coupling of electrogenic cells to graphene devices — Michael Sejer Wismer, Felix Rolf, Damia Viana, •Martin Lottner, Lucas Hess, and Jose A. Garrido — Walter Schottky Institut - Technische Universität München, Am Coulombwall 4, 85748 Garching

In this contribution, we will demonstrate the electrical coupling between electrogenic cells and graphene-based solution-gated field effect transistors (SGFETs). To this end, HEK293 and HL1 cells were cultured on 8x8 arrays of graphene SGFETs with feature sizes of 10 mu x 20 mu. Graphene was grown by chemical vapour deposition (CVD) on copper foil and transferred to sapphire substrates, on which field effect transistors were fabricated using standard semiconductor technology. The devices show a typical maximum transconductance of >100 muS at 0.1 V drain-source voltage. This value is stable over months of storage. HEK293 cells were used to analyse the electrical coupling between cells and transistors. A model considering the distribution of ions within the cell transistor cleft and ion sensitivity of the graphene SGFETs fits the measured signals very well. Additionally, nano-transistors were defined by e-beam lithography, which allowed feature sizes down to 50 nm. With these nanoscale devices a signal-to-noise ratio of 2.5 could be obtained within single recordings of HL1 activity. Analysis of the measured ionic currents allowed to draw conclusions about local inhomogeneities of ion channel concentration within the membrane. Further, experiments for the stimulation of PC12 cells using arrays of graphene SGFET and graphene-based microelectrode arrays (MEAs) are under preparation.

DY 39.11 Thu 17:45 POT 081

Graphene solution-gated field effect transistors on flexible substrates — •Andrea Bonaccini Calia, Benno M. Blaschke, Lucas H. Hess, Max Seifert, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Graphene based solution-gated field effect transistors (SGFETs) hold great promise for biosensors and bioelectronic applications. Due to its unique combination of electronic, mechanical, and chemical properties, such as high charge carrier mobility, flexibility and good biocompatibility, graphene has been shown to be an excellent material for sensing in electrolyte environments. Sensors based on graphene SGFETs have already been realized on rigid substrates for various analytes, as well as for the detection of cell signals. However, this technology hold some severe problems for biomedical and in vivo applications. One of the major problems is the rigidity of the substrate itself, which does not allow a proper mechanical matching to the biological tissue, resulting in the formation of scar tissue. Therefore, flexible devices are currently considered as a major step towards the development of more biocompatible implants. In this work, an array of graphene SGFETs is fabricated on a flexible polymer substrate. We present a detailed electrical characterization of the flexible graphene SGFETs in electrolyte and compare their performance to graphene SGFETs on rigid substrates. In addition, we analyze the effect of changes in the electrolyte's pH and ionic strength on the transistor performance and present a model to explain the obtained results. Furthermore, the low-frequency noise performance of graphene devices on flexible substrates is discussed.

DY 40: Poster - Quantum Systems/ Stat. Phys./ Diffusive Process

In this poster session there are contribution to the topics
- Quantum Systems
- Statistical Physics
- Diffusive Processes

Time: Thursday 17:00–19:00 Location: P3

DY 40.1 Thu 17:00 P3

Global structure of regular tori in a generic 4D symplectic map — Steffen Lange[1,2], Martin Richter[1,2], •Franziska Onken[1], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]Institut für Theoretische Physik, TechnischeUniversität Dresden, 01062 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany

We progress towards an understanding of the phase-space structures of higher-dimensional systems similar to the well-known case of Hamiltonian systems with two degrees of freedom. Using 3D phase-space slices and frequency analysis we investigate the global organization of regular tori of a generic 4D symplectic map with a mixed phase space. We visualize how all of the regular 2-tori are organized around a skeleton of elliptic 1-tori in the 4D phase space. The 1-tori occur in two types of one-parameter families: The first type are Lyapunov families attached to elliptic-elliptic periodic orbits. These families are observed to exist even far away from their periodic orbit and beyond major resonance gaps. We explain how the second type originates from rank-1 resonances. At resonance gaps of both families either (i) periodic orbits exist, similiar to the Poincaré-Birkhoff theorem for 2D maps, or (ii) the family forms large bends. In combination these results allow for describing the self-similiar hierarchy of regular tori in the 4D phase space.

DY 40.2 Thu 17:00 P3

Trapping of chaotic orbits in 4D symplectic maps — •Steffen Lange[1,2], Martin Richter[1,2], Arnd Bäcker[1,2], and Roland Ketzmerick[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany

Generic Hamiltonian systems with more than two degrees of freedom lead to chaotic zones in phase space which are all interconnected by the Arnol'd web. We study 4D symplectic maps with a regular region embedded in a large chaotic sea, i.e., far away from the near-integrable regime. Chaotic orbits are trapped in the vicinity of the regular region and show a power-law decay of survival times. We search for the trapping mechanism by visualizing the trapped orbits in 3D phase-space slices of the 4D phase space and analyzing their time-dependent frequencies. We find that the underlying mechanism is clearly different from trapping in 2D maps and not related to the Arnol'd web. Instead, an anisotropic diffusion near the surface of the regular region is observed. In this surface region the chaotic orbits are frequently trapped at different resonances.

DY 40.3 Thu 17:00 P3

Perturbative analysis of whispering-gallery modes in the Limaçon microcavity — •Marcus Kraft and Jan Wiersig — Otto-von-Guericke-Universität Magdeburg, 39016 Magdeburg

In recent experiments it has been demonstrated that wavelength-scale microdisk lasers with the shape of a Limaçon can support high-quality whispering-gallery modes despite the chaotic internal ray dynamics. Here, we show that these modes can be accurately described by a perturbation theory for slightly deformed microdisk cavities. Our results reveal that the performance of the perturbation theory can be considerably improved by a suitable choice of the origin around which the perturbation series is expanded.

DY 40.4 Thu 17:00 P3

Experiments with Superconducting Microwave Billiards — •Barbara Dietz, Maksim Miski-Oglu, Tobias Klaus, Christo-

pher Cuno, and Achim Richter — Institut für Kernphysik, TU-Darmstadt, Schlossgartenstr. 9, D-64298 Darmstadt

We present experimental results on spectral properties of Dirac billiards simulating graphene billiards. They consist of a photonic crystal enclosed in a microwave billiard. Here we use the analogy between the associated scalar Helmholtz equation and the Schrödinger equation and the fact that the peculiar properties of graphene are solely due to the symmetry properties of its hexagonal lattice structure. We will present results on the spectral properties and length spectra of periodic orbits that were obtained in high precision experiments with superconducting Dirac billiards. Furthermore we determined the density of states with an unprecedented accuracy and investigated the effect of edge states on its features. It exhibits two sharp peaks at the frequencies of the van Hove singularities. There, a topological transition from the relativistic Dirac regime to the non-relativistc Schrödinger regime takes place which can be identified with a neck-disrupting Lifshitz and with an excited state quantum phase transition. The theoretical considerations are corroborated by experimental results on the features of the density of states.

*Supported by the Deutsche Forschungsgemeinschaft (DFG) within the Collaborative Research Center SFB634.

DY 40.5 Thu 17:00 P3

Aufbau und Spektrale Eigenschaften einen Mikrowellenanalogon des Fulleren Moleküls — •Tobias Klaus, Barbara Dietz und Achim Richter — Institut für Kernphysik, TU-Darmstadt

Wir präsentieren die Realisierung einen Mikrowellenanalogon der C60 Fullerene Molekül.

DY 40.6 Thu 17:00 P3

Modelliernug von einem C_{60} Fullerenmolekül durch einen supraleitenden Mikrowellenresonator — Barbara Dietz, •Tobias Klaus, Maksim Miski-Oglu, Achim Richter, Tetyana Skipa und Marcus Wunderle — TU Darmstadt, Schlossgartenstr. 9, 64289 Darmstadt

Wir präsentieren unsere Untersuchung zu den spektralen Eigenschaften eines C_{60} Fullerenmoleküls mit einem supraleitenden Mikrowellenresonator, einem sogenannten Fullerenbillard. Dies ist ein Mikrowellenresonator, dessen Hohlraum die Form eines C_{60} Fullerenmoleküls hat. Hierzu wurden in eine Vollkugel 60 Kreisresonatoren und 90 Wellenleiter, die diese miteinander verbinden, eingefräst. Das Index Theorem wurde mit Hilfe des Fullerenbillards experimentell untersucht. Dieses verbindet die Anzahl der Eigenzustände mit Eigenwert Null mit der Topologie der Oberfäche von C_{60}. Um ein vollständiges Eigenfrequenzspektrum zu erhalten, wurde ein supraleitendes Mikrowellenbillard verwendet, dessen Güten Werte von $Q > 10^5$ erreichen.

Gefördert durch die DFG im Rahmen des SFB 634.

DY 40.7 Thu 17:00 P3

Spektrale Eigenschaften eines Chaotischen Mikrowellen Africa Diracbillard — Barbara Dietz, Tobias Klaus, Maksim Miski-Oglu, Achim Richter, Tetyana Skipa und •Marcus Wunderle — TU-Darmstadt,Schlossgartenstr. 9, 64289 Darmstadt

Wir präsentieren die experimentelle Untersuchung der spektralen Eigenschaften eines supraleitenden Mikrowellen Diracbillards. Die Form des Billards entspricht den Umrissen des Kontinents Afrika und wird deshalb Afrika Diracbillard genannt. Das Mikrowellenbillard enthält Metallzylindern, die einen photonischen Kristall mit der Struktur eines Dreiecksgitters bilden. In der Nähe einer bestimmten Frequenz, der sogenannten Diracfrequenz, ist die Dispersionsrelation der elektromagnetische Wellen ähnlich der von masselosen, relativistischen Fermionen und wird durch die Diracgleichung beschrieben. Der Einsatz von supraleitenden Billards ermöglicht die experimentelle Bestimmung eines vollständigen Spektrums von Eigenfrequenzen. Die Fluktuationseigenschaften folgen der Vorhersage der Zufallsmatrizen Theorie für ein GOE Ensemble.

Gefördert durch die DFG im Rahmen des SFB 634.

DY 40.8 Thu 17:00 P3

Two-level dynamics in presence of a band-gapped material — •Martin Pietsch, Denis Kast, and Joachim Ankerhold — Institut für Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm

We studied the dynamics of a single spin that interacts with a bosonic broadband reservoir (spin boson model). The spectrum is Ohmic, but with a gap near a certain frequency. Our numerically exact Path Integral Monte Carlo simulations, including recent extensions [1,2], reveal that the spectral hole imprints its frequency onto the dynamics, thereby prohibiting the fixation of a well-defined coherent-incoherent transition point for increasing system-reservoir coupling. This investigation is motivated by impressive progress in designing photonic bandgap materials during the last years.

[1] D. Kast and J. Ankerhold, Phys. Rev. Lett. 110, 010402 (2013).
[2] D. Kast and J. Ankerhold, Phys. Rev. B 87, 134301 (2013).

DY 40.9 Thu 17:00 P3

All-electric qubit control in heavy hole quantum dots via non-Abelian geometric phases — •Dietrich Rothe[1], Jan Budich[3], Hartmut Buhmann[2], Ewelina Hankiewciz[1], and Björn Trauzettel[1] — [1]Instit. für theoret. Physik, Universität Würzburg — [2]Physikal. Institut, Universität Würzburg — [3]Department of Physics, Stockholm University, Sweden

We demonstrate how non-Abelian geometric phases can be used to universally process a spin qubit in heavy hole quantum dots in the absence of magnetic fields. A time dependent electric quadrupole field is used to perform any desired single qubit operation by virtue of non-Abelian holonomy. During the proposed operations, the degeneracy of the time dependent two level system representing the qubit is not split. Since time reversal symmetry is preserved and hyperfine coupling is known to be weak in spin qubits based on heavy holes, we expect very long coherence times in the proposed setup.

Published in Phys. Rev. B 85, 205425 (2012). We acknowledge support by the DFG within SPP1285 (HA5893/1-2 and BU1113/3-2).

DY 40.10 Thu 17:00 P3

Coherent dynamics of a quantum spin coupled to a fermionic bath — •Lars-Hendrik Frahm, Benjamin Baxevanis, and Daniela Pfannkuche — I. Institut für Theoretische Physik, Universität Hamburg, Germany

We investigate the dynamics of a quantum spin system weakly coupled to its environment. The environment is modeled by a bath of fermions coupled by exchange interaction to the spin system. Partial polarization of the fermionic bath affects the spin dynamics and we investigate its impact on the precession and coherence of the spin system. In order to determine the coherent dynamics of the spin system coupled to the bath, we calculate the time evolution of coherent states, i.e. off-diagonal density matrix elements. This is achieved by employing the time-convolutionless projection operator technique which allows for the computation of the coherent, non-Markovian spin dynamics.

DY 40.11 Thu 17:00 P3

Efficient Implementation and Application of the Artificial Bee Colony Algorithm to Low-Dimensional Optimization Problems — •Guido Falk von Rudorff[1], Christoph Wehmeyer[1], and Daniel Sebastiani[1,2] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institute of Chemistry, Martin-Luther-Universität Halle-Wittenberg, von-Danckelmann-Platz 4, 06120 Halle, Germany

We adapt a swarm-intelligence-based optimization method (the artificial bee colony algorithm, ABC) for the prediction of global minima on potential energy surfaces of molecular geometries to enhance its parallel scaling properties and to improve the escaping behavior from deep local minima. Specifically, we apply the approach to the geometry optimization of Lennard-Jones clusters. We illustrate the performance and the scaling properties of the parallelization scheme for several system sizes (5-20 particles) and different atomic interaction potentials. Deriving optimal parameters for the algorithm is a highly non-trivial problem. We present a strategy for finding ranges of the parameters of the ABC algorithm which yield maximal performance for Lennard-Jones clusters and Morse clusters. We evaluate small carbon clusters using the Tersoff potential to illustrate which kind of potential energy surfaces can be searched with this algorithm in a timely manner. The suggested parameter ranges turn out to be very similar for these different interaction potentials; thus, we believe that our reported values are fairly general for the ABC algorithm applied to chemical optimization problems.

DY 40.12 Thu 17:00 P3

Spontaneous imbibition in microfluidic pores — •Zeinab Sadjadi[1], Michael Jung[2], Heiko Rieger[1], and Ralf Seemann[2] — [1]Theoretical Physics Department, Saarland University, Saarbrucken, Germany — [2]Experimental Physics Department, Saarland University, Saarbrucken, Germany

Recently, spontaneous imbibition of wetting liquids in porous media consisting of elongated pores, has been studied theoretically [1,2]. The numerical simulation as well as analytical model predict that at a pore junction, meniscus propagation can come to a 'halt' for a certain amount of time. These 'arrest events' lead to a fast broadening of the imbibition front in the porous medium. Here we study this phenomenon in a single junction of three microfluidic pores and present experimental evidence for 'halt' of meniscus for the first time.

[1] S. Gruener, Z.Sadjadi, H.E. Hermes, A. V. Kityk, K. Knorr, S. U.Egelhaaf, H. Rieger and P. Huber, Proc. Natl. Acad. Sci. U. S. A. 109, 10245 (2012)

[2] Z. Sadjadi and H. Rieger, Phys. Rev. Lett.110, 144502 (2013)

DY 40.13 Thu 17:00 P3

Stiff Directed Lines in Random Media — •Horst-Holger Boltz and Jan Kierfeld — TU Dortmund, Dortmund, Deutschland

We investigate the localization of stiff directed lines with bending energy by a short-range random potential. Using perturbative arguments, Flory arguments, and a replica calculation, we show that a stiff directed line in 1+d dimensions undergoes a localization transition with increasing disorder for d>2/3. We demonstrate that this transition is accessible by numerical transfer matrix calculations in 1+1 dimensions and analyze the properties of the disorder-dominated phase. On the basis of the two-replica problem, we propose a relation between the localization of stiff directed lines in 1+d dimensions and of directed lines under tension in 1+3d dimensions, which is strongly supported by identical free energy distributions. This shows that pair interactions in the replicated Hamiltonian determine the nature of directed line localization transitions with consequences for the critical behavior of the Kardar-Parisi-Zhang (KPZ) equation. Furthermore, we quantify how the persistence length of the stiff directed line is reduced by disorder.

DY 40.14 Thu 17:00 P3

Polymer Adsorption onto a Stripe-Patterned Surface — •Momchil Ivanov[1], Monika Möddel[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig — [2]Basycon Unternehmensberatung, München

Previous theoretical studies have provided phase diagrams that lay the foundations for a better understanding of the basic mechanisms of polymer adsorption. This particular study focuses on a single polymer chain in a confined volume and its adsorption onto a stripe-patterned surface.

A minimalistic simple-cubic lattice model was used where the chain is represented by an interacting self-avoiding walk (ISAW) and was confined between an attractive patterned wall and a steric wall with no interaction whatsoever. The pattern consisted of parallel stripes of defined width and separation. Besides the pattern parameters, three energy scales determine the phase diagram of the system: chain-surface attraction, chain-pattern attraction and chain self-attraction.

Chains of lengths up to $N = 19$ monomers were studied using the method of exact enumeration. The influence of the energy scales and pattern parameters on the system was analysed with the help of temperature vs. chain-pattern attraction phase diagrams. These diagrams were constructed by means of both canonical and microcanonical analysis of the enumeration data.

DY 40.15 Thu 17:00 P3

Steady-State Droplet Size Distributions for Breath Figures with Dripping — •Jakob de Maeyer[1,2], Johannes Blaschke[1,2], and Jürgen Vollmer[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation (MPIDS), 37077 Göttingen, Germany — [2]Fakultät für Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

The concept of condensing droplets on a surface (breath figures) plays a crucial role in microfabrication and high-efficiency heat transfer.

Recent studies have shown that existing scaling theories fail to explain experimental data on the droplet size distribution. A faithful description must explicitly deal with growth mechanisms of the smallest droplets and their fractal packing. The fractal droplet arrangement introduces non-trivial and non-universal scaling exponents.

Here, we show that the arising of the non-universal exponents is related to the breakdown of a common approximation in Smoluchowski models of droplet aggregation: there is no simple decomposition of the coalescence kernel into single-particle distribution functions.

We revisit these findings in the light of new experimental data on steady states where droplets are constantly removed from the surface through gravity-induced dripping.

DY 40.16 Thu 17:00 P3

Mesoscopic Model for Topological Defect in Nematic Liquid Crystals — •Kuang-Wu Lee and Marco G. Mazza — MPI für Dynamik und Selbstorganisation, 37077 Göttingen, Deutschland

Topological line defects in nemetic liquid crystals under flow has been investigated in microfluidic channels [Sengupta et al. 2013]. To study the dynamical nature of this topological defect and its shear flow/nematic elasticity interactions under different flow regimes, we develop a mesoscopic scheme based on the stochastic rotational dynamics (SRD) method. We adapt the SRD method to particles with orientational degree of freedom. The model is tested for the liquid crystal phase transition under different temperatures. The viscosity and rotational diffusion coefficients, usually assigned in fluid approach, are self-generated in this model, hence this mesoscopic model enables us to study the local transport due to flow.

DY 40.17 Thu 17:00 P3

Rate of Mutual Information Between Coarse-Grained Non-Markovian Variables — •David Hartich, Andre C. Barato, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Germany

Mutual information, a central quantity in information theory, quantifies correlations between two random variables. We focus on bipartite systems with two coarse-grained processes that together specify a continuous time Markov process. In this case no analytical formula for the rate of mutual information is known. However, we calculate an upper bound on the rate of mutual information that becomes exact in some special cases with time scale separation. Additionally, we develop a numerical method to calculate the rate of mutual information in continuous time. We illustrate our main results with simple four state models, which provide insight into the relation between the rate of mutual information and the thermodynamic entropy production.

[1] A. C. Barato, D. Hartich, and U. Seifert, J. Stat. Phys. **153**, 460 (2013)

[2] A. C. Barato, D. Hartich, and U. Seifert, Phys. Rev. E **87**, 042104 (2013)

DY 40.18 Thu 17:00 P3

Fluctuation Spectra and Coarse Graining in Stochastic Dynamics — •Artur Wachtel[1,2], Bernhard Altaner[1,2], and Jürgen Vollmer[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation (MPI DS), Göttingen — [2]Fakultät für Physik, Georg-August-Universität, Göttingen

Fluctuations in small biological systems can be crucial for their function. Large-deviation theory characterizes such rare events from the perspective of stochastic processes.

In most cases it is very difficult to directly determine the large-deviation functions. Circumventing this necessity, I present a method to quantify the fluctuation spectra for arbitrary Markovian models with finite state space. Under non-equilibrium conditions, current-like observables are of special interest. The space of all current-like observables has a natural decomposition into orthogonal complements. Remarkably, the fluctuation spectrum of any observable is entirely determined by only one of these components.

The method is applied to study differences of fluctuations in setups sampling the same dynamics at different resolutions. Coarse graining relates these models and can be done in a way that preserves expectation values of observables. However, the effects of the coarse graining on the fluctuations are not obvious. These differences are explicitly worked out for simple model systems.

DY 40.19 Thu 17:00 P3

Generalized Bose condensation into multiple states and heat transport in tight-binding lattices far from equilibrium — •Alexander Schnell[1,2], Daniel Vorberg[1,2], Waltraut Wustmann[1,2], Roland Ketzmerick[1,2], and André Eckardt[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, 01062 Dresden, Germany

If an ideal Bose gas is driven into a steady state far from equilibrium, then a generalized form of Bose condensation can occur [1]. Namely the single-particle states unambiguously separate into two groups: one, that we call Bose selected, whose occupations increase linearly when the total particle number is increased at fixed system size, and

another one whose occupations saturate. We study this effect in a tight-binding lattice, where the non-equilibrium regime is achieved either by coupling the system to two heat baths, one of positive and another one of negative temperature, or by a combination of periodic forcing and the coupling to a heat bath. We investigate which and how many single-particle states are selected in such lattice systems. We, moreover, address how system properties like the heat conductivity are controlled by the various parameters of the model, like lattice size, dimensionality, or the coupling to the heat bath(s).

[1] D. Vorberg, W. Wustmann, R. Ketzmerick and A. Eckardt, Phys. Rev. Lett. (to be published), arXiv:1308.2776

DY 40.20 Thu 17:00 P3

Generalized Bose-Einstein condensation into multiple states in driven-dissipative systems — •Daniel Vorberg[1,2], Waltraut Wustmann[1,2], Roland Ketzmerick[1,2], and André Eckardt[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, 01062 Dresden, Germany

Bose-Einstein condensation, the macroscopic occupation of a single quantum state, appears in equilibrium quantum statistical mechanics and persists also in the hydrodynamic regime close to equilibrium. Here we show that even when a degenerate Bose gas is driven into a steady state far from equilibrium, where the notion of a single-particle ground state becomes meaningless, Bose-Einstein condensation survives in a generalized form: the unambiguous selection of an odd number of states acquiring large occupations. Within mean-field theory, we derive a criterion for when a single and when multiple states are *Bose selected* in a non-interacting gas. We study the effect in several driven-dissipative model systems, and propose a quantum switch for heat conductivity based on shifting between one and three selected states.

DY 40.21 Thu 17:00 P3

Nonthermal Fixed Points and Superfluid Turbulence in Ultracold Bose Gases — Sebastian Erne[1,2], •Markus Karl[1,2], Steven Mathey[1,2], Boris Nowak[1,2], Andreas Samberg[1,2], Jan Schole[1,2], Carlo Ewerz[1,2], and Thomas Gasenzer[1,2] — [1]Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg — [2]ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt, Germany

Turbulence appears in situations where, e.g., an energy flux goes from large to small scales where finally the energy is dissipated. As a result the distribution of occupation numbers of excitations follows a power law with a universal critical exponent. The situation can be described as a nonthermal fixed point of the dynamical equations. Single-particle momentum spectra for a dynamically evolving Bose gas are analysed using semi-classical simulations and quantum-field theoretic methods based on effective-action techniques. These give information about possible universal scaling behaviour. The connection of this scaling with the appearance of topological excitations such as solitons and vortices in one-component gases and domain walls and spin textures in multi-component systems is discussed. In addition, this results are discussed from the point of view of holographic superfluids. The results open a view on solitary wave dynamics from the point of view of critical phenomena far from thermal equilibrium and on a possibility to study non-thermal fixed points and superfluid turbulence in experiment without the necessity of detecting solitons and vortices in situ.

DY 40.22 Thu 17:00 P3

Nonlinear Response in the Driven Lattice Lorentz Gas — •Sebastian Leitmann[1,2] and Thomas Franosch[1,2] — [1]Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Technikerstraße 25/2, A-6020 Innsbruck, Austria — [2]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

We determine the nonlinear time-dependent response of a tracer on a lattice with randomly distributed hard obstacles as a force is switched on [1]. The calculation is exact to first order in the obstacle density and holds for arbitrarily large forces. Whereas, on the impurity-free lattice, the nonlinear drift velocity in the stationary state is analytic in the driving force, interactions with impurities introduce logarithmic contributions beyond the linear regime. The long-time decay of the velocity toward the steady state is exponentially fast for any finite value of the force, in striking contrast to the power-law relaxation predicted within linear response. We discuss the range of validity of our analytic results by comparison to stochastic simulations.

[1] Sebastian Leitmann and Thomas Franosch, Phys. Rev. Lett. 111, 190603 (2013).

DY 40.23 Thu 17:00 P3

Diffusion of nanorods on quasicrystalline substrates with phasonic drift — •Felix Rühle[1], Michael Schmiedeberg[2], and Holger Stark[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf

In order to understand ordering and growth on quasicrystalline substrates, experiments and theory have investigated colloidal ordering in a two-dimensional decagonal potential that is realizable by laser interference patterns [1,2]. In particular, spheres and rods show interesting phase behaviour and colloidal dynamics [2,3].

Phasons are hydrodynamic modes that occur in quasiperiodic crystals only and represent local rearrangements of atoms. In this contribution, we apply a phasonic drift with a constant drift velocity to the decagonal potential [4]. We place single nanorods of two different lengths in the potential and investigate their diffusive motion for different phasonic drift velocities. The results are obtained using kinetic Monte-Carlo simulations. We observe that single rods pass through a superdiffusive regime before reaching normal diffusion in the long-time limit. Depending on the length of the rods and the direction of the phasonic drift, they may align themselves with a preferential direction in real space.

[1] J. Mikhael et al., *Nature*, **454**, 501 (2008).
[2] M. Schmiedeberg and H.Stark, *PRL*, **101**, 218302 (2008).
[3] P. Kählitz, M. Schoen, and H. Stark, *JCP*, **137**, 224705 (2012).
[4] J.A. Kromer et al., *EPJE*, **36**, 25 (2013).

DY 40.24 Thu 17:00 P3

Computersimulation of colloidal particles in channel geometries — •Ullrich Siems, Birte Heinze, and Peter Nielaba — University of Konstanz

We present the results of Brownian Dynamics Simulation of colloidal particles confined to two- and three-dimensional micro-channels under the influence of external forces. Counter-flow in three dimensions and the influence of a periodic substrate potential in two dimensions are under investigation. Confinement into channels can have a great influence on diffusion and transport properties in such systems.

DY 40.25 Thu 17:00 P3

The impact of interactions on the rotational ratchet effect in magnetic colloidal suspensions — •Teresa Reinhard and Sabine H. L. Klapp — Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

The extraction of directed motion from undirected random motion is a well-known problem with many different applications, such as the efficiency of heat engines, biological transport or nano-motors.
To analyze such effects, we consider a system of dipolar colloids with dipole-dipole interactions that are driven out-of-equilibrium by an oscillating magnetic field. Due to microscopic Brownian motion, these systems can exhibit directed rotational motions without an externally applied net torque [1]. This so-called ratchet effect is analysed on basis of the dynamical density functional theory [2].
Specifically, we investigate the impact of the frequency of the external field, as well as the dependence on the distance vector between the particles.
We compare our results with those from a mean-field Fokker-planck approach [3] and from particle-based computer simulations [4].

[1] A. Engel and P. Reimann, Phys. Rev. Let. 91, 060602 (2003).
[2] M. Rex, H. H. Wensink and H. Löwen, Phys Rev E 76, 021403 (2007)
[3] V. Becker and A. Engel Phys. Rev. E 75, 031118 (2007).
[4] S. Jäger and S. H. L. Klapp, Phys. Rev. E 86, 061402 (2012).

DY 40.26 Thu 17:00 P3

Ageing and nonergodicity in the Standard map — •Tony Albers and Günter Radons — Technische Universität Chemnitz, Germany

We investigate diffusion processes occurring in the phase space of the well-known Standard map, which is a paradigmatic example for low-

dimensional non-integrable Hamiltonian chaos. These diffusion processes deviate from the laws of normal diffusion and especially have non-stationary increments. As a consequence, statistical quantities depend on the elapsed time (ageing time) between the beginning of the process and the beginning of the measurement. Furthermore, ergodicity of these processes can be broken in the sense that ensemble and time averages do not coincide and time averages become random variables. We study the ageing and nonergodicity of the observed anomalous diffusion in terms of the mean squared displacement and the distribution of generalized diffusivities [1], which describes the fluctuations during the diffusion process around the generalized diffusion coefficient that is obtained from the asymptotic time dependence of the mean-squared displacement.
[1] T. Albers and G. Radons, EPL 102, 40006 (2013)

DY 40.27 Thu 17:00 P3

Universality of Anomalous Transport in Model Crowded Media — •Markus Spanner[1], Felix Höfling[2], Gerd Schröder-Turk[1], and Thomas Franosch[1,3] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]MPI für komplexe Systeme, Stuttgart, and IV. Institut für Theoretische Physik, Universität Stuttgart, Germany — [3]Institut für Theoretische Physik, Leopold-Franzens-Universität Innsbruck, Austria

The Lorentz model is a simple model for transport in porous materials, where a point-like tracer moves through an array of random overlapping spheres. At the point where the void space between the frozen-in obstacles undergoes a percolation transition, sub-diffusive transport $\delta r^2(t) \sim t^{2/d_w}$, $d_w = 4.81$ can be observed. In this regime transport is dominated by narrow channels in the host structure, where the tracer can barely squeeze through.

With our simulations, we want to test the influence of these narrow channels, a) by introducing correlations in the obstacle positions, thereby changing the statistics of channel widths, and b) by comparing ballistic and Brownian tracer dynamics, i.e. changing the way channels are probed by the tracer.

While in the first case, the system is stable and d_w stays unchanged, in the second case, a splitting in two universality classes can by observed.

DY 40.28 Thu 17:00 P3

Anomalous transport of self-propelled particles in biological environments — Mohammadreza Shaebani, •Zeinab Sadjadi, Heiko Rieger, and Ludger Santen — Theoretical Physics Department, Saarland University, Saarbrucken, Germany

We study the influence of structural characteristics of random filamentous networks – or equivalently the stepping strategy in continuous space – on the transport properties of a random walker. A general master equation formalism is developed to investigate the persistent motion of self-propelled particles, which enables us to identify the key parameters and disentangle their contributions to the transport properties. Depending on the persistency of the walker and the anisotropy and heterogeneity of the structure, the particles exhibit an anomalous diffusive dynamics. We establish the existence of up to three different regimes of motion, and determine the phase diagrams of the behavior. We verify that the crossover times between different regimes as well as the long-term diffusion coefficient can be enhanced by a few orders of magnitude within the biologically relevant range of control parameters. The analytical predictions are in excellent agreement with simulation results.

DY 40.29 Thu 17:00 P3

Collective behaviour of self-propelled particles with nematic alignment in three dimensions — •Rebekka Heyn and Marco G. Mazza — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany

In the field of active swimmers, numerical models with simple, local interaction rules are a powerful instrument to study collective phenomena of any type of self-propelled particles.

Here, we fill the gap of such a model in three dimensions with local nematic alignment and study the collective behaviour in large systems (up to 10^6 particles in reasonable computational time). The system shows interesting collective states such as global nematic order, isotropic phase, coexistence of different phases, and density waves. We investigate these waves in detail, as they show a surprising symmetry breaking of the nematic interaction. Moreover, we examine the effects of spatial disorder by adding obstacles to the system. We study their influence on the collective behaviour of the self-propelled particles and, specifically, on the waves.

DY 40.30 Thu 17:00 P3

Statistical analysis of trajectories of sedimenting beads in a active fluid — •Levke Ortlieb, Matthias Mussler, Christian Wagner, and Thomas John — Universität des Saarlandes, Experimentalphysik 7.2, 66123 Saarbrücken, Germany

Aqueous suspensions of life-forms have existed on earth since the very beginning of life. All cellular life is characterized by metabolism and requires a continuous assimilation of food or light as its energy source. Locomotion favors the admission of these materials and raises survival probability.

Here we present details on an experimental setup to investigate the locomotion of the green alga chlamydomonas reinhardtii and in particular the sedimentation of micro-spheres of different diameters in a Hele-Shaw-flow environment. The alga has two flagella, a diameter of 10 μm and swims as a puller with approximately 50 μm/s. We present extracted statistical properties of the suspended, passive bead positions, e.g. the mean square displacement or the probability density function of positions. We will compare our results from the microswimmer suspensions with the Brownian motion characteristics of sedimenting particles in very dilute systems and the characteristics in passive sedimenting particles at higher volume concentrations. In our microswimmer suspensions as well as in the sedimentation at higher volume concentrations, the hydrodynamic interaction becomes important and a non-Brownian behavior can be observed.

DY 40.31 Thu 17:00 P3

Investigating Chlamydomonas reinhardtii's gears of motion by means of holographic optical tweezers and micropipettes — •Christian Ruloff, Thomas John, and Christian Wagner — Dynamics of Fluids, Wagner Group, Saarland University

Chlamydomonas reinhardtii (CR) is an approximately twelve micron sized unicellular green algae which uses two beating flagella for locomotion. The light-sensing eyespot is used to detect the incident light and stears its motion to control the distance between the algae itself and the light source for ideal photosynthesis: At low light intensities the algae is swimming towards the light source while at strong illumination CR increases its distance to it. Both flagella are not beating in the same plane leading to a superposition of foreward movement with a slight rotation mandatory for phototaxis. Besides the wild type there exist many mutants like blind or deflagellated ones. Therefore, CR is used as a model organism for research on basic questions like "How do cells move?" or "How do cells respond to light?". Using holographic optical tweezers (HOT) we generate two counterrotating optical vortices at the same spatial position which form a cogwheel potential whose radius is chosen to match the algae's body size. With this technique it is possible to partially suppress out-of-plane movement of the CR to reduce the problem to two dimensions. This is necessary because with our setup it is only possible to observe movements in the focal plane of the microscope objective. Furthermore, we want to compare our results for an almost free-swimming CR with measurements of CR in a totally body-fixed state when held by a micropipette.

DY 40.32 Thu 17:00 P3

Phase field modelling of oxide scale growth — •Fabian Twiste[1], Claas Hüter[1], Robert Spatschek[1], Jörg Neugebauer[1], and Michael Finnis[2] — [1]Max-Planck Institut für Eisenforschung, Düsseldorf — [2]Imperial College, London

We present recent steps towards a phase field description of oxide scale growth for the modelling of corrosion processes and the formation of protective layers in high-temperature applications. In the model we consider chemical reactions which are taking place both at the scale-air surface as well as at the scale-metal interface. Charged defects therefore play a central role, and their equilibrium distributions and diffusion through the oxide layer is influenced by external and self-generated electrostatic fields. The phase field framework for the description of the film growth is therefore supplemented by reaction-diffusion equations and consideration of the local electrical potential. The predictions are compared against sharp interface considerations.

DY 40.33 Thu 17:00 P3

Light sensitivity of Belousov-Zhabotinsky reaction with 1,4-cyclohexanedione as the organic substrate — Andreas Bindler and •Stefan C. Müller — Institute of Experimental Physics, Otto-von-Guericke-Universität Magdeburg

The study of spatio-temporal patterns in chemically reactive systems is one of the central problems of modern reaction kinetics. A well-known experimental model system is the Belousov-Zhabotinsky (BZ) reaction, which exhibits oscillations and chemical waves. In a photosensitive Ru-catalyzed version of this reaction light can act as an external control of various features of such patterns. Recent work is focused on the light-sensitivity of 1,4-cyclohexadione (CHD) as a new substrate, which has particular advantages and specific properties of interest. We study the influence of CHD and its intermediates on the kinetics of the BZ-reaction and on other chemical reagents like the catalyst or bromide. The response to illumination of the BZ-reaction with CHD is much more complex, compared with the previously investigated light-sensitive reaction including Ruthenium and malonic acid as the substrate. Thus, we have investigated the pattern evolution in the presence of CHD and different catalysts. A major goal is to determine, how the interaction between CHD and Ruthenium under irradiation in the visible spectrum can be minimized.

DY 41: Poster - Pattern/ Nonlinear Dyn./ Fluids/ Granular/ Critical Phen.

In this poster session there are contribution to the topics
- Pattern Formation
- Nonlinear Dynamic Effects
- Fluids/ soft matter / granular
- Critical Phenomena

Time: Thursday 17:00–19:00 Location: P3

DY 41.1 Thu 17:00 P3

Formation of salt polygons on salt playas — •Antoine Fourrière and Lucas Goehring — Max Planck Institut for Dynamics and Self-organization, Göttingen, Germany

On the grounds of natural salt deserts or in evaporation pools for industrial salt extraction, one can see some self-organized polygonal network of 1-2m diameter. The edges of these periodic structures are formed by salt crystal ridges, that is the reason why we call them 'salt polygons'. In this work, we analyze three different potential mechanisms to explain the formation and the scaling of salt polygons: (i) dessication cracks, (ii) non-linear wrinkling of an elastic layer and (iii) porous medium convection cells in the soil. We built a 2D experiment to test these ideas and most particularly the third one. A Hele-Shaw cell is filled with a porous medium saturated with a salty solution and heated from the side. Surface evaporation causes a steady upward flow of salty water, which leads to precipitation near the surface. Hence, a vertical salt gradient builds up in the porous medium and causes a overturning of denser saltier water. An appropriate Rayleigh number (cf. Lapwood 1948) controls the onset of convection in the porous medium. We change the Rayleigh number by varying the evaporation rates or the permeability of the model soil and measure the wavelength of the salt features that form at the surface. We also visualize the water movements into the Hele-Shaw cell during the experiment. Finally, by using our experimental observations, we revisit the natural formation of these patterns with a pinch of salt.

DY 41.2 Thu 17:00 P3

Growth of Hair Ice — •Christina Inninger[1], Lorenz Eichler[1], Christian Mätzler[2], and Thomas Grillenbeck[1] — [1]Ignaz-Günther-Gymnasium Rosenheim, Rosenheim, Germay — [2]University of Bern, Institute for Applied Physics, Switzerland

The hair-like or cotton-like ice formations known as hair ice are sometimes to be observed on rotten and humid beech wood or oak. Its origin is not quite clear. The supposition that an active fungus causes the growth to the strange phenomenon rests on some physical and wooden-anatomical facts: Saprophytic fungi feed on organic nutrients which they diminish enzymatically. The end products CO_2 and H_20 as well as some warmth originate during the enzymatic degradation of starch and fat stored in the wooden body above all the wooden rays. The gas pressure of the CO_2 expels the water stored in the wooden body as well as the water produced in the degeneration process through the radial channels of the rays to the wood surface. On the surface it freezes at temperatures slightly below melting point due to the crystallization germs. We study the growth process and distinguish hair ice from related forms, such as ice ribbons and needle ice.

DY 41.3 Thu 17:00 P3

Phenomenological simulations of metal layer formation during sputter deposition — •Sven-Jannik Wöhnert[1], Gunthard Benecke[1,2], Matthias Schwartzkopf[1], and Stephan V. Roth[1] — [1]DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Am Mühlenberg 1 OT Golm, D-14476 Potsdam, Germany

Sputter deposition is one high-throughput method to install with highest rates patterned nanostructures on surfaces. Grazing incidence small-angle X-ray (GISAXS) scattering nowadays delivers a wealth of information during in-situ processes and real-time observations [1,2]. To analyze the data, simulation of GISAXS pattern based on realspace structures is indispensable. Based on the results of [1], we therefore simulate the in-situ experiments by continuous deposition of gold atoms on a silicon surface and follow their arrangement into clusters using Monte-Carlo methods. As boundary conditions, we impose the successful geometric model of [1]. Therefore, we are able to image the cluster layer built-up during the continuous depostion of Au atoms during the sputter process. We present quantitative visualization of the different growth modes of the real-time experiment. Especially we are able to observe coalescence, contact angle and diffusion on the nanoscale.

[1] Schwartzkopf et al., Nanoscale 5, 5053-5062 (2013)
[2] Shun et al., J. Phys. Chem. Lett., 3170-3175 (2013)

DY 41.4 Thu 17:00 P3

Non-equilibrium dynamics of ordered modulated phases — •Christian Riesch, Günter Radons, and Robert Magerle — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

We have performed numerical simulations of simple models for modulated phases, with the focus on 2D stripe-forming systems. The system is initially prepared in an ordered state without topological defects, and the subsequent evolution at a finite noise strength is monitored. This results in a rich non-equilibrium dynamics. In particular, we find aging in the two-time correlation function of the local stripe orientation, which is explained in terms of a growing correlation length perpendicular to the stripes. We also discuss the effects of system size, aspect ratio and a possible cross-over to 1D behavior.

DY 41.5 Thu 17:00 P3

Optical birefringence in dried laponite films — •Pawan Nandakishore, Anupam Sengupta, and Lucas Goehring — Max Planck Institute for Dynamics and Self-Organization (MPIDS)

The emergence of anisotropy in a material can be attributed to either the structure of the materials or the buildup of internal stresses within a material. Using Optical polarization microscopy we study dried laponite suspensions under ambient conditions. We observe birefringence in the bulk and on the edges of dried laponite films. Laponite is know to transition from an isotropic liquid to an isotropic gel and finally to a nematic gel as a function of the initial concentration and changing salinity. We observe that dried samples of laponite are birefringent even when the laponite concentration before drying is in the isotropic gel phase regime. The birefringence scales with concentration before drying and reaches a maximum when it is in the nematic phase regime. Bulk birefringence in the dried samples can be attributed to ordering of laponite disks due to drying where as the birefringence in the edge is stress induced. We observe similar stress induced birefringence at edges of a crack opening and along the edge of laponite thick

films (millimeter-centimeters films). Dried laponite films are model systems to study stress induced birefringence and birefringence due to structural anisotropy.

DY 41.6 Thu 17:00 P3

Stability of Binary Patterns in Optomechanical Arrays — •Christian Brendel, Roland Lauter, Steven Habraken, Max Ludwig, and Florian Marquardt — Institute for Theoretical Physics, Friedrich-Alexander University, Staudtstraße 7, 91058 Erlangen, Germany

We focus on two-dimensional arrays of mechanically coupled, laser-driven, optomechanical cells. Consisting of both an optical mode and a mechanical (vibrational) mode, those cells can be driven into self-sustained oscillations. A non-linear set of differential equations, that describe the evolution of the phases thereof, can be derived [1]. The parameters of this classical model can be tuned by the laser drives. We concentrate on binary patterns in which all oscillators are initialized to phases of 0 or pi. Being fixpoints of the equations of motion, the stability of these configurations is observed in limiting cases of the model. Moreover, we study the stability and time evolution of domain configurations within binary patterns and give an overview of the effects occurring in the parameter space.

[1] G. Heinrich, M. Ludwig, J. Qian, B. Kubala and F. Marquardt, Phys. Rev. Lett. 107, 043603 (2011)

DY 41.7 Thu 17:00 P3

Functional connectivity of distant cortical regions: role of remote synchronization and network symmetry — •Philipp Hövel[1,2] and Vesna Vuksanović[1,2] — [1]Technische Universität Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Germany

We aim to reproduce resting-state functional-connectivity (FC) networks modeling (neural and BOLD) activity of the interacting cortical regions. We focus on the topology of the network interactions as a main ingredient of our model based on experimental data taking into account both anatomical and functional connectivity. Hence, important information about the presence/absence of direct neural connections within functionally connected nodes is included in the model. Controlling for direct neural links in functional networks allows us to test hypothesis that remote synchronization of the neural activity, arising from the underlying topology of the network interactions, accounts for the FC between distant cortical regions.

Using Kuramoto oscillators with frequencies in gamma frequency range, we explore emergence of the synchronization between pairs of the neural network nodes for different interactions topologies obtained via thresholds to the empirically derived FC matrix. We show that pronounced synchrony between nodes reflects symmetry of the coupling matrix, i.e., the strong overlap in the respective neighborhoods. We also illustrate that symmetry of the interactions drives remote nodes into synchronized activity and therefore plays central role in emergence of the functional connections between distant cortical regions.

DY 41.8 Thu 17:00 P3

Aging in systems of classical oscillators — •Florin Ionita, Darka Labavić, and Hildegard Meyer-Ortmanns — School of Engineering and Science, Jacobs University Bremen, PO Box 750561, D-28725 Bremen, Germany

Aging is a familiar phenomenon from glassy systems, in particular from spin glasses and materials with slow relaxation processes after a perturbation, breaking of time-translation invariance, and dynamical scaling. We study these effects in systems of classical oscillators, active rotators and Kuramoto oscillators that are coupled with frustrated bonds. The induced multiplicity of attractors of fixed-point or limit cycle solutions leads to a rough potential landscape. When the system is exposed to additive noise, the oscillator phases migrate through this landscape and escape from one metastable state to another, generating a multitude of different escape times [1]. When the system is quenched from the regime of a unique fixed point towards the regime of multistable limit-cycle solutions, the autocorrelation functions depend on the waiting time after the quench and show dynamical scaling for an intermediate regime of time periods between the two measurements. We point out parallels between oscillatory systems and spin glasses in the physical origin of aging.

[1] F. Ionita, D. Labavić, M. Zaks, and H. Meyer-Ortmanns, Order-by-disorder in classical oscillator systems, Eur. Phys. J. B (2013), in press.

DY 41.9 Thu 17:00 P3

Heteroclinic snaking near a heteroclinic chain in dragged meniscus problems — •Mariano Galvagno[1], Dmitri Tseluiko[1], and Uwe Thiele[1,2] — [1]Department of Mathematical Sciences, Loughborough University, UK — [2]Institut für Theoretische Physik, Universität Münster, Germany

We study the deposition of a non-volatile liquid film onto a flat heated inclined plate extracted from a bath at constant speed. We analyse steady-state meniscus solutions of a 2d long-wave mesoscopic hydrodynamic description that incorporates wettability via a Derjaguin (disjoining) pressure as the plate velocity is changed. We observe snaking behaviour when the plate inclination angle is above a certain critical value. Otherwise, the bifurcation curve is monotonic. The solutions along these curves are characterised by a foot-like structure [1] formed close to the meniscus. The foot is preceded by a thin precursor film further up the plate. We show that the snaking is related to the existence of infinitely many heteroclinic orbits close to a heteroclinic chain in an appropriate 3d phase space connecting the fixed points of the system [2]. [1] A. Münch, P.L. Evans, Phys. D 209, 2005. [2] M. Galvagno, D. Tseluiko, U. Thiele, arxiv.org/abs/1307.4618

DY 41.10 Thu 17:00 P3

Effects of empowerment-driven spins in the 2D-Ising model — •Lukas Everding[1] and Daniel Polani[2] — [1]Ludwig-Maximilians-Universität, München/Deutschland — [2]University of Hertfordshire, Hatfield/UK

Recent work has increasingly focussed on large-scale non-equilibrium systems. Especially interesting are systems which are pushed away from equilibrium by active ("driven") particles where the driving forces may arise from various principles. We specifically investigate large-scale systems with particles driven by a principle belonging to the class of 'intrinsic motivation' drives called "empowerment". Empowerment-driven particles are given a limited freedom of choice in their behavior and they act with the goal of getting the largest possible perceivable influence onto the system, basically maximizing an information-theoretic criterion for combined controllability/observability. We investigate the effects of seeding a 2-d Ising model with a small number of empowerment-driven particles: using Monte-Carlo methods, we first show that these particles stabilize the system at finite magnetization, even well above the critical temperature. The system is dragged away from the unordered equilibrium state and kept in a more ordered state. Second, we show that the second-order phase transition of the classical Ising model at T_c is smoothed out to a slow and gradual transition from the ordered state to the unordered one with increasing temperature. An analogous effect is seen in a quite different Nagel-Schreckenberg model which indicates that empowerment-driven particles seem to push the bounds of ordered regimes into the disordered regimes.

DY 41.11 Thu 17:00 P3

How Markovian is a time series? — •Pedro Lencastre[1,2], Frank Raischel[3], and Pedro G. Lind[4] — [1]ISCTE-IUL, Av. Forças Armadas, 1649-026 Lisboa, Portugal — [2]Mathematical Department of Faculdade de Ciências of University of Lisbon, Campo Grande 1749-016 Lisboa — [3]Instituto Dom Luiz, CGUL, 1749-016 University of Lisbon, Lisbon, Portugal — [4]ForWind and Institute of Physics, Carl-von-Ossietzky University of Oldenburg, DE-26111 Oldenburg, Germany

We describe a simple procedure for testing if a series of measurements is non-markovian or not for a particular time-lag. Our procedure is based in a quantitative measure of non-markovianity and is particular suited for short time series. The error of the test can be estimated. Further, we briefly discuss how to apply this procedure to real data in geophysics and interdisciplinary topics.

DY 41.12 Thu 17:00 P3

Multi-point description and time series reconstruction — •Ali Hadjihosseini — ForWind, Oldenburg,Germany

We proposed a method that allows a reconstruction of time series based on multi-point statistics given by hierarchical process. This method is able to model water wave time series including extreme events. We extend the stochastic cascade description by conditioning on wave height value itself, and find that the corresponding process is also governed by a Fokker-Planck equation, which contains as a leading term a simple additional wave height-dependent coefficient in the drift function. As a main result it is shown that this method is able to reproduce the extreme events in time series.

DY 41.13 Thu 17:00 P3

Wind Farm Optimization with Monte Carlo Methods — •Klaus Nagl and Ingo Morgenstern — Universität Regensburg

We determine the optimal layout of the turbines inside a wind farm, taking the wake effects into account. We show the differences between the N.O Jensen and the Larsen Wake Models.

For this purpose we use a simulated annealing algorithm adapted to this specific problem. Two different objective functions are considered: the Annual Energy Production and the Profit, which lead to different optima. A detailed analysis is presented to help determining the best objective function to choose in each case.

DY 41.14 Thu 17:00 P3

Bayesian Analysis of Non-Gaussian Long-Range Dependent Processes — Tim Graves[5], •Nicholas Watkins[1,2,3,4,8], Bobby Gramacy[6,5], and Christian Franzke[7,8] — [1]MPIPKS, Dresden, Germany — [2]CFSA, Physics, University of Warwick, Coventry, UK — [3]MCT, Open University, Milton Keynes, UK — [4]CATS, LSE, London, UK — [5]Statistics Laboratory, University of Cambridge, Cambridge, UK — [6]Booth School of Business, The University of Chicago, Chicago, USA. — [7]Meteorologisches Institut, Universität Hamburg, Germany — [8]British Antarctic Survey, Cambridge, United Kingdom

We have used MCMC algorithms to perform a Bayesian analysis of Auto-Regressive Fractionally-Integrated Moving-Average ARFIMA(p, d, q) processes, which are capable of modeling LRD [Graves, Ph.D, 2013]. Our principal aim is to obtain inference about the long memory parameter, d, with secondary interest in the scale and location parameters. We have developed a reversible-jump method enabling us to integrate over different model forms for the short memory component. We initially assume Gaussianity, and have tested the method on both synthetic and physical time series. We have extended the ARFIMA model by weakening the Gaussianity assumption, assuming an α-stable distribution for the innovations, and performing joint inference on d and α. We will present a study of the dependence of the posterior variance of the memory parameter d on the length of the time series considered. This will be compared with equivalent error diagnostics for other measures of d.

DY 41.15 Thu 17:00 P3

Simulating single-molecule pulling experiments: coupling transport and molecular dynamics simulations — •Alessandro Pirrotta[1], Ignacio Franco[2], and Gemma C. Solomon[1] — [1]Nano-Science Center and Department of Chemistry, University of Copenhagen, 2100, Copenhagen Ø, Denmark — [2]Department of Chemistry, University of Rochester, Rochester, NY 14627-0216 USA

We aim to develop a method that would allow us to simulate single-molecule pulling experiments using molecular dynamics (MD) simulations coupled to transport. In order to do this, we have worked to extend the force field employed in the MD simulation to explore a wider range of molecules. The DFTB+ code is employed to compute the transmission function for the system and simulate the electrical properties, in order to investigate correlations between the conformational changes of a molecular system and the conductance. In particular, we apply this to a hydrogen-bonded dimer with a range of bonding motifs as the system is extended.

DY 41.16 Thu 17:00 P3

POCLMD: A Flexible GPU Accelerated Molecular Dynamics Code — •Chuanfu Luo[1] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

Recently, heterogeneous computing becomes a trend in high performance computing. Many newly built super-computers are equipped with powerful GPUs or coprocessors, which can deliver up to 5 Tflops per unit. The OpenCL is an open standard programing language which is supported by all vendors of GPU or coprocessor. Code written in OpenCL can run on multiple-core CPUs, GPUs, and coprocessors without any changes. POCLMD is designed to be a fast, flexible and easy-to-use MD code, which is programed in Python and OpenCL through PyOpenCL [1]. All time-consuming calculations are performed on GPU, and CPU only deals with data transfer and pre-/post- processing. The first released version of POCLMD will support basic simulations of NVE/NVT/NPT for coarse-graining polymeric models, including bond, angle and pair-wised LJ potentials. Further potentials of dihedral and long-range electric interactions will be supported later. The performance of POCLMD can catch up >80% of HOOMD-blue [2] (the fastest CUDA based MD code as we know) on the same NVIDIA's GPUs. POCLMD on one AMD's HD7970 card runs 60-80 times faster than LAMMPS on a single core Q6600 CPU (2.4GHz).

[1] http://mathema.tician.de/software/pyopencl
[2] http://codeblue.umich.edu/hoomd-blue/

DY 41.17 Thu 17:00 P3

Importance of asymmetry for cross-streamline migration of bead spring models in oscillating shear flows — •Matthias Laumann, Diego Kienle, and Walter Zimmermann — Theoretische Physik, Universität Bayreuth, 95440 Bayreuth, Germany

We investigate cross-streamline migration of bead-spring polymers in time-dependent linear shear flows in the limit of small Reynolds numbers. Dumbbells and ring polymers are used as base models and it is shown that cross-streamline migration in time-dependent linear shear flow exists only if the deformable dumbbell or the ring polymer have an intrinsic asymmetry. Once the asymmetry being in place, the migration efficiency can be controlled by adjusting the amplitude and the period of the oscillating shear gradient. Our findings suggest that small deformable objects of different asymmetry and elasticity may be separated by switched shear flows via the process of cross-streamline migration.

DY 41.18 Thu 17:00 P3

Dynamics of Bound States in a real-valued Swift-Hohenberg Equation induced by Delayed Feedback — •Felix Tabbert and Svetlana Gurevich — Institut für theoretische Physik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 9, 48149 Münster

We are interested in the stability-properties of stationary bound state solutions of the real-valued Swift-Hohenberg Equation, subjected to time-delayed feedback. We show that the change in delay-time and delay-strength leads to various dynamical solutions including the formation of travelling waves, labyrinth-like patterns, as well as moving and rotating bound states.

We provide a linear stability analysis of the delayed system and obtain an analytical expression for the delay-induced instability-threshold. Numerical calculations are also carried out, showing good agreement with the analytical predictions.

DY 41.19 Thu 17:00 P3

Quasiperiodic and chaotic motion of active particles in Poiseuille flow — •Igor Dudas, Andreas Zöttl, and Holger Stark — TU Berlin

Active particles have an intrinsic propulsion mechanism which constantly keeps them out of equilibrium. They swim with a constant velocity while the swimming direction can be manipulated by an external field. In this contribution we demonstrate that an active particle swimming in Poiseuille flow exhibits typical nonlinear dynamics mainly driven by the cross-streamline migration due to activity [1,2]. Our model system can be mapped onto a Hamiltonian system equivalent to the nonlinear pendulum. Bounding surfaces introduce dissipation while swimmers in Poiseuille flow with elliptic cross section exhibit quasiperiodic and chaotic behavior depending on the flow velocity and initial conditions.

[1] A. Zöttl and H. Stark, Phys. Rev. Lett. **108**, 218104 (2012).
[2] A. Zöttl and H. Stark, Eur. Phys. J. E **36**, 4 (2013).

DY 41.20 Thu 17:00 P3

Vorticity distributions in two dimensional forced turbulence — •Markus Blank-Burian — Institut für Physikalische Chemie, WWU Münster, Deutschland

In statistical fluid dynamics, turbulent flows can be characterized by probability density functions (PDFs). Within the framework of the Lundgren-Monin-Novikov hierarchy, one can derive time evolution equations for the PDFs as summarized in [1]. The closure problem arises herein by coupling multi-point PDFs of different order. These equations can also be rewritten using conditional averages.

Until now, the PDFs have been approximated by gaussian distributions. Looking at numerical data, one finds that the shape of the vorticity PDF and also the conditional averages over the vorticity field depend strongly on the strength of the forcing. The shape of the one-point as well as the two-point PDF can be modeled by a convolution of two multivariate stable distributions.

As a result of this, one can describe the force dependence of the

one-point conditonal average of the vorticity field as an interpolation between a strongly oscillating function and a smooth function. It turns out, that the former function is associated with a gaussian distribution and can be attributed to the forcing. It dominates at small vorticity strength around $\omega < 2\sigma$. The other function is associated with a lorentz distribution and dominates clearly at large vortices $\omega > 5\sigma$.

[1] Friedrich,Daitche,Kamps,Lülff,Voßkuhle,Wilczek: The Lundgren-Monin-Novikov Hierarchy: Kinetic Equations for Turbulence, C. R. Acad. Sci

DY 41.21 Thu 17:00 P3

Evolution equations for two dimensional elliptic shaped gaussian vortices — •Markus Blank-Burian — Institut für Physikalische Chemie, WWU Münster, Deutschland

The easiest model to describe two dimensional vortices in turbulent flows is the point vortex model. This model has an inherent problem, as it can not describe either attraction or repulsion of two vortices. By studying numerical and experimental data, one can see, that in first approximation two interacting vortices maintain a nearly elliptic gaussian shape for a rather long time. Vortices with the same sign attract each other and orientate themselves parallel with an angle of approximately 45° to their connecting vector. Vortices with different sign orient themselves nearly perpendicular to each other while moving in the same direction.

Based on an idea in [1], one can derive equations of motion for two interacting elliptically shaped gaussian vortices, describing their evolution in time. This model then correctly predicts attraction and repulsion of two vortices, depending on the strenth and orientation of the vortices. The characteristic angles of 45° are found stable as well. The famous Lamb-Oseen vortex is contained as a limiting case of symmetric shape.

[1] Friedrich, Friedrich: Generalized vortex-model for the inverse cascade of two-dimensional turbulence, http://arxiv.org/abs/1111.5808

DY 41.22 Thu 17:00 P3

Fluctuations of orientational order and clustering in a two-dimensional colloidal system under quenched disorder — •Tobias Horn[1], Sven Deutschländer[2], Hartmut Löwen[1], Georg Maret[2], and Peter Keim[2] — [1]Institut für Theoretische Physik II: Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany — [2]Fachbereich für Physik, Universität Konstanz, D-78464 Konstanz, Germany

Using both, video-microscopy of superparamagnetic colloidal particles confined in two dimensions and computer simulations of repulsive parallel dipoles, we study the formation of fluctuating orientational clusters and topological defects with respect to the KTHNY-like melting scenario under quenched disorder. We analyze cluster densities, average cluster sizes, the population of non-cluster particles as well as the development of defects as a function of system temperature and disorder strength. In addition, a probability distribution of clustering and orientational order is presented. We find that the well known disorder-induced widening of the hexatic phase can be traced back to the distinct characteristics of clustering and defect formation along the melting transitions from the solid phase via the hexatic phase to the isotropic fluid.

DY 41.23 Thu 17:00 P3

Packing of hard spheres in cylinders and applications — •Adil Mughal[1], Denis Weaire[2], Ho Kei Chan[2], and Stefan Hutzler[2] — [1]Institut fur Theoretische Physik, Friedrich-Alexander Universitat Erlangen-Nurnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]School of Physics, Trinity College, Dublin 2, Republic of Ireland

We study the optimal packing of hard spheres in an infinitely long cylinder. Our simulations have yielded dozens of periodic, mechanically stable, structures as the ratio of the cylinder (D) to sphere (d) diameter is varied. Up to D/d=2.715 the densest structures are composed entirely of spheres which are in contact with the cylinder. The density reaches a maximum at discrete values of D/d when a maximum number of contacts are established. These maximal contact packings are of the classic "phyllotactic" type, familiar in biology. However, between these points we observe another type of packing, termed line-slip.

An analytic understanding of these rigid structures follows by recourse to a yet simpler problem: the packing of disks on a cylinder. We show that maximal contact packings correspond to the perfect wrapping of a honeycomb arrangement of disks around a cylindrical tube. While line-slip packings are inhomogeneous deformations of the honeycomb lattice modified to wrap around the cylinder.

Beyond D/d=2.715 the structures are more complex, since they incorporate internal spheres. We review some relevant experiments with hard spheres, small bubbles and discuss similar structures found in nature. We discuss the chirality of these packings and potential applications in photonics.

DY 41.24 Thu 17:00 P3

Ab-initio Calculations Show which Metal Melts are Simple Liquids — •Felix Hummel[1], Jeppe Dyre[2], Georg Kresse[1], and Ulf Pedersen[1,3] — [1]University of Vienna, Austria — [2]Roskilde University, Denmark — [3]Technical University of Vienna, Austria

Simple liquids or strongly correlated liquids (SCL) exhibit identical thermodynamical behaviour up to unit scaling for states on isomorph curves. Melting lines and lines of constant excess entropy follow isomorph curves for simple liquids.

We performed ab-initio calculations for all metal melts at the triple point, testing the degree of isomorphic behaviour. We find that most melts are indeed simple to a high degree, at least at PBE-DFT level.

We also show that an inverse-power-law (IPL) model - forming fully correlated liquids - gives an excellent approximation for retrieving thermodynamic properties of the simple metal melts. For those metals, the IPL approximation even allows to predict the ambient pressure crystal structure solely from liquid data.

DY 41.25 Thu 17:00 P3

Shapes of branched polymer networks — •Christian von Ferber[1] and Marvin Bishop[2] — [1]AMRC, Coventry University, Coventry, UK — [2]Department of Computer Science and Mathematics, Manhattan College, New York, USA

We investigate the shapes of polymer networks embedded in two- and three-dimensional space as function of their architecture. To this end we employ both analytical methods as well as the Monte Carlo pivot algorithm to investigate continuum, tangent hard-sphere branched polymers both in the ideal and the excluded volume regimes.

The mean square radius of gyration, the g-ratio, and the form factors are evaluated. The MC data agree well with the exactly determined form factors. The form factors reveal the influence of the polymer structure at short distances.

DY 41.26 Thu 17:00 P3

A hydrodynamic approach to driven granular systems — •Mathias Hummel, James Clewett, and Marco G. Mazza — Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Deutschland

We study a hydrodynamic approach to vibrated granular gases. We use a modification of the compressible Navier-Stokes equation in 3D. To handle the shockwaves in our simulations we use high-order WENO methods and the Multi-Stage approach(MUSTA) flux is used to calculate the convective fluxes. The integrations in our finite-volume method is performed through Gaussian integration points. Our results are compared with molecular dynamics simulations. We study and characterise the shockwaves traveling through the system and the nonequilibrium pattern that emerges in the steady state.

DY 41.27 Thu 17:00 P3

Vertically vibrated granular gas with van der Waals Interactions — •Qiong Bai, James P. D. Clewett, and Marco G. Mazza — Max Plank Intstitute for Dynamics and Self-Organization, Bunsen Str. 10, 37073 Goettingen, Germany

As a classical thermodynamic non-equilibrium system, granular matter is still a field full of unexplored static and dynamic behaviour. Here we focus on a vertically vibrated granular system. We also consider van der Waals interactions between particles. By means of molecular dynamics simulations, we study and characterize the different phase separations that emerge from the interplay of dissipative and conservative interactions. We observe new states with intriguing dynamics.

DY 41.28 Thu 17:00 P3

Scaling of Wet Particle Collisions — •Thomas Müller, Ingo Rehberg, and Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

For the description of natural phenomena like debris flow or the formation of planetary rings as well as for the development of industrial applications, a thorough knowledge about the dynamics of granular matter is crucial. In many of these systems, the surfaces of the in-

teracting particles are covered with a thin liquid film. Consequently, compared to the description of dry systems, additional energy losses due to the wetting liquid have to be taken into account.

We investigate macroscopic spheres bouncing on a flat surface that is covered with a liquid film. The coefficient of normal restitution e_n, defined as the ratio between the relative rebound and impact velocity of a binary impact is used to characterize the amount of energy dissipation during the collision. Our primary goal is to understand how various parameters, such as impact velocity, particle and liquid properties, influence e_n. Experiments with glass spheres have already shown, that e_n can be rescaled with the Stokes number which depends on the ratio between inertia forces and viscous forces, as long as the ratio between sphere size and liquid film thickness is kept constant. Here, we present further experimental results with spherical particles of different materials, in order to test the universality of such a scaling behavior and to understand the associated energy dissipation mechanisms.

DY 41.29 Thu 17:00 P3

Contact angle hysteresis of an evaporizing droplet: control with inkjet printing — Simeon Völkel, Thomas Müller, Ingo Rehberg, and •Kai Huang — Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany

Wetting is ubiquitous in nature and of tremendous importance in industries such as mining, enhanced oil recovering, pharmaceutics, painting, and inkjet printing. Understanding the dynamics of wetting, such as contact angle hysteresis and pinning of the three phase contact line, can help to enhance the efficiency of various applications. Toward this goal, the challenge arises from the fact that most real life wetting phenomena are not in thermodynamic equilibrium. For example, the evaporation of a drop on a flat surface may lead to various drying patterns.

Here, we focus on the evaporation of a water drop on a surface of various materials and measure associated change of contact angle and drop size. In addition to evaporation, we employ an inkjet printing device to control the volume of the drop with an accuracy of nanoliter, in order to investigate the hysteresis of the contact angle and related pinning of the contact lines. It is found that the contact angle decays linearly with time during evaporation, provided that the contact line is pinned. In case of a smooth Polytetrafluoroethylene (PTFE) surface, the depinning drop shrinks with a fixed contact angle of around 90 degrees. Possible mechanisms accounting for such a phenomenon will be discussed.

DY 41.30 Thu 17:00 P3

Measuring contact forces in 3D inside granular packing — •Junaid M. Laskar[1], Stephan Herminghaus[1], Matthias Schröter[1], and Karen E. Daniels[2] — [1]Dynamics of Complex Fluids, Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Department of Physics, North Carolina State University, Raleigh, USA

Knowing the contact forces and their statistical distributions inside a granular packing is a central question in granular physics. Measurement of contact force distributions and force chains till now have been possible only in 2D [1,2]. However, measurement inside a 3D granular packing, where the physics is expected to be different, still remains an experimental challenge.

An intrinsic property of ruby is linear change of its fluorescence signal as a function of applied stress [3]. By making use of this property, an experimental technique is developed to measure contact forces inside the packing of ruby spheres. The results obtained by this technique, which is based on aplanatic solid immersion lens optics and two photon fluorescence spectroscopy, will be discussed.

References: [1] T. S. Majumdar and R. P. Behringer, Nature 453, 1079 (2005) [2] Karen E. Daniels and Nicholas W. Hayman, J. of Geophys. Res. 113, B11411 (2008) [3] Y. Chen et al., J. Appl. Phys. 101, 084908 (2007)

DY 41.31 Thu 17:00 P3

Structural and mechanical properties of random packings of spherocylinders: a simulation study — •Pascal Wieland and Claus Heussinger — Georg-August-Universität Göttingen, Institut für Theoretische Physik

An energy-minimization technique is developed to study random packings of soft spherocylinders in the vicinity of the jamming point.

We are interested in structural and mechanical properties as a function of the aspect ratio of the cylinders. In particular, we determine the average number of inter-particle contacts as well as their types (side-side, tip-side, tip-tip).

The simulation data is compared with experimental results obtained from x-ray tomography of spaghetti packings (in collaboration with C. Lewandowski and M. Schröter, also see their contribution).

DY 41.32 Thu 17:00 P3

How do spaghetti make contacts? — •Cyprian Lewandowski[1,3], Christian Brosowski[2], Max Neudecker[1], Claus Heussinger[2], and Matthias Schröter[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — [2]Institute of Theoretical Physics, University Goettingen, 37077 Goettingen, Germany — [3]Department of Physics, Imperial College London, SW7 2AZ London, United Kingdom

The aim of this study was to understand stability of random packings of cylinders based on an analysis of inter-particle contacts. Three aspect ratios (L) of cylinders were prepared from uncooked spaghettini strands. Samples were compacted with a vertical shaking apparatus and data was gathered using X-ray microtomography. Image analysis was carried out with algorithms implemented in MATLAB, achieving precision of length fit better than 0.5%. The scaling of the average global contact number with packing fraction was observed to follow the asymptotic scaling relation $\phi L = \text{constant}$ [Philipse 1996]. By carrying out a nearest-neighbour transformation, Voronoi cells for each particle were obtained. These are the first measurements that allow to elucidate the relation between local contacts and local packing fraction.

DY 41.33 Thu 17:00 P3

Plant roots growing in granular media: intelligent penetrators? — •Caroline Bauer[1,4], Rebecca Liese[2], Ina Christin Meier[2], Kai Huang[3], and Matthias Schröter[1] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen — [2]Albrecht-von-Haller-Institut für Pflanzenwissenschaften, Universität Göttingen — [3]Experimentalphysik V, Universität Bayreuth — [4]Institut für Experimentelle Physik, Universität Magdeburg

A root growing in the soil viewed from a granular physics perspective is a penetration experiment, where the tip of the root exerts shear stress on the granular medium at its front. Depending on its initial packing fraction, disordered granular matter subjected to shear either compacts (low packing fraction), dilates (high packing fraction) or does not change its packing fraction (dilatancy onset). The differences of root growth to a classical penetration experiment are a certain flexibility of the root and, more importantly, the involvement of a living organism that underwent an evolutionary process.

Thus the question we want to address is the following: Do roots grow in a different way when they encounter dense vs. loose granular material, and if so, does the transition happen at the point of dilatancy onset? To answer this question we plant seeds of Sinapis alba L. in a cell filled with a monodisperse granular aggregate. They are grown in a climate chamber where they are kept moist continuously with a modified Hoagland's solution. The growth of the roots and the changes in the granulate are monitored by regular scans with an X-ray tomograph.

DY 41.34 Thu 17:00 P3

Statitistics of 2D granular assemblies comprised of polygonal particles — •Volker Becker and Klaus Kassner — Institut für theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Germany

A possible approach for the statistical description of granular assemblies is Edwards assumption that all blocked states which occupy the same volume are equally probable[1]. Assemblies prepared by the same process, result to packages of the same volume fraction, except fluctuations. In the context of Edwards theory the dependency of the fluctuation strengths on the volume fraction is linked to the compactivity by a granular version of fluctuation dissipation theorem. Provided that the fluctuation strength is a function of the mean volume only one can compute the compactivity by measuring the fluctuations. We performed computer simulations using two dimensional polygonal particles excited periodically by short acceleration pulses and found that the volume fraction is a non-monotonic function of the pulse strength. This allows us to test whether or not the fluctuations are a function of the volume fraction only or not. In the second case an extended version of Edwards theory, containing the angoricity tensor as second state variable, has to be considered[2]. We will calculate the compactivity and if necessary the angoricity. We will compare the results with assemblies prepared by a different process on an otherwise iden-

tical systems. Due to Edwards theory, the results should only depend on the granular state variables, but not on details of the protocol. [1] Physica A 157, 1080 (1989) [2] PRL 109,238001 (2012)

DY 41.35 Thu 17:00 P3

Contemplating coincidences: Rigorous testing for synchrony between event-related time series — •Reik V. Donner[1,2] and Jonathan F. Donges[2,3] — [1]Max Planck Institute for Biogeochemistry, Jena, Germany — [2]Potsdam Institute for Climate Impact Research, Potsdam, Germany — [3]Stockholm Resilience Centre, Stockholm University, Sweden

Studying temporal point processes like the timings of extreme events is a common problem in various fields of sciences. When series of distinct types of events are available in a common time frame, assessing their statistical interrelationships can be valuable for testing theories proposing specific causal relationships. Here, we introduce a simple statistical framework for computing the probability that the observed number of simultaneous events in two series is due to chance. While in the case of rare events and no serial correlations, this probability can be well approximated analytically, introducing short- or long-range correlations as typical in real-world data can result in substantial deviations from this theory. We systematically study these deviations based on numerical results for some generic stochastic processes as well as real-world examples related to climate and ecosystem variability. Formal links to other techniques like Ripley's cross-K function from spatial statistics, or event synchronization and cross-recurrence rate from nonlinear time series analysis are briefly addressed.

DY 41.36 Thu 17:00 P3

Loop Percolation with non standard critical behavior — •Matthias J. F. Hoffmann, Susan Nachtrab, Gerd E. Schröder-Turk, and Klaus Mecke — Friedrich-Alexander-Universität Erlangen-Nürnberg

Loop percolation refers to a wide class of percolation models, that change the coordination of randomly selected vertices, rather than deleting bonds or sites. Bond and site percolation are included as special cases. Starting from a regular fully connected network each node is split with probability p. By introducing asymmetry into the splitting process the percolation threshold and the percolation critical exponents can be changed. The two dimensional square lattice and the three dimensional diamond lattice are shown as examples for this model class, each exhibiting different critical behavior to the stardard universality class of bond/site percolation.

DY 41.37 Thu 17:00 P3

Percolation threshold on planar Euclidean Gabriel Graphs — •Christoph Norrenbrock — Carl-von-Ossietzky Universität Oldenburg

Planar proximity graphs such as the Gabriel Graph (GG) [1] are of potential interest in the context of wireless ad hoc networks, since the embedded edges provide proximity information regarding their adjacent nodes. Furthermore, the edge-sets ensure that the graph is connected, i.e. nodes are able to communicate to each other via intermediate ones. Using the highly efficient, union-find based algorithm by Newman and Ziff [2], we simulate the bond and site-percolation problem on planar Gabriel graphs of size $N = 1024$ to $N = 36864$ (N refers to the number of nodes) for Poisson point processes. Previously, it has already been shown that non-trivial percolation thresholds exist and rough estimates for their location has been made [3]. By means of finite-size-scaling techniques, we determine the precise location of the bond and site percolation thresholds and deduce the common percolation critical exponents from the GG data. The associated universality class is that of standard $2D$ percolation.

[1] Gabriel and Sokal, Systematic Biology 18, 259 (1969)
[2] Newman and Ziff, Phys Rev. Lett. 85, 4104 (2000)
[3] Bertin, Billiot, Drouilhet, Adv. Appl. Prob. 34, 689 (2002)

DY 41.38 Thu 17:00 P3

Kinetic Growth Random Walks — •Johannes Bock, Niklas Fricke, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, 04009 Leipzig, Germany.

Random walks are investigated since the 1950s and there are quite a number of different models for them, e.g. the self-avoiding walk and the kinetic growth walk. Here the kinetic growth walk is investigated in comparison to existing and up-to-date knowledge and results for the self-avoiding walk. These comparisons were done on regular lattices as well as on diluted lattices including the limiting case of percolation clusters where fractal properties become important.

DY 41.39 Thu 17:00 P3

Domain growth and coarsening of liquid droplets in vapor medium in a phase separating van der Waals fluid with SPH in three dimensions — •Martin Pütz and Peter Nielaba — University of Konstanz, Department of Physics, 78457 Konstanz, Germany

We study the dynamics of liquid-vapor phase separation of a van der Waals fluid induced by homogeneous nucleation and in later stage the domain growth and coarsening process towards equilibrated systems. Therefore we performed simulations in three dimensions with Smoothed Particlel Hydrodynamics (SPH) which provides the possibility to follow the dynamics through different time scales. The coexistence region and hence the process of homogeneous nucleation arises naturally by the implementation of the well known van der Waals equation as an equation of state and by a thermal conduction equation.

DY 41.40 Thu 17:00 P3

Melting of 2D solids under quenched disorder — •Sven Deutschländer[1], Tobias Horn[2], Hartmut Löwen[2], Georg Maret[1], and Peter Keim[1] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

We investigate the effect of quenched random disorder on the melting transition of two-dimensional solids providing both colloidal experiments and monte carlo simulations of parallel repulsive dipols [1]. According to the KTHNY theory, we observe a two step melting process with an intermediate hexatic phase and studying the orientational order and correlation, we are able to investigate the detailed phase behavior for weak disorder strengths. By determining orientational correlation times and Frank's constant, we show that the solid-hexatic phase transition is strongly influenced by pinning, while the hexatic-isotropic transition remains rather unaffected. This is in agreement with theoretical predictions for solids with quenched random disorder, first discussed by D. R. Nelson and later by M.-C. Cha and H. A. Fertig. In addition, we observe critical-like orientational fluctuations on large time scales. These fluctuations are consistent with the continuous nature of the phase transitions and not locally affected by quenched disorder .

[1] S. Deutschländer, T. Kruppa, H. Löwen, G. Maret, and P. Keim, Phys. Rev. Lett. 111, 098301 (2013)

DY 41.41 Thu 17:00 P3

Transmuted finite-size scaling at first-order phase transitions with exponential degeneracy of ordered states — •Marco Mueller[1], Wolfhard Janke[1], and Desmond A. Johnston[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — [2]Department of Mathematics, School of Mathematical and Computer Sciences, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS, Scotland, UK

We note that the standard inverse system volume scaling for finite-size corrections at a first-order phase transition (i.e. $1/L^3$ for an $L \times L \times L$ lattice in $3D$) is transmuted to $1/L^2$ scaling if there is an exponential low-temperature phase degeneracy. The gonihedric Ising model which has a four-spin interaction, plaquette Hamiltonian provides an exemplar of just such a system. We use multicanonical simulations of this model to generate high-precision data which provides strong confirmation of the transmuted finite-size scaling law. The dual to the gonihedric model, which is an anisotropically coupled Ashkin-Teller model, has a similar degeneracy and also displays the transmuted scaling.

DY 41.42 Thu 17:00 P3

Information-theoretic analysis of ground-state phase transitions for 2D and 3D frustrated spin systems — •Oliver Melchert and Alexander K. Hartmann — Universität Oldenburg

We consider standard information-theoretic observables [1] to analyze ground-state spin configurations for disordered and frustrated model systems. More precisely, we address the 2D random bond Ising model and the 3D random field Ising ferromagnet, which both exhibit a continuous transition from an ordered to a disordered ground state as a model parameter is varied [2]. The ground-state configurations for both setups can be obtained in polynomial time via exact combinatorial optimization algorithms.

By computing the three observables entropy, i.e. a measure of disorder, excess entropy and multi-information, i.e. measures of complexity,

it is possible to detect changes in the spatial structure of the ground states as the respective critical point is approached. The finite-size scaling behavior of the information-theoretic observables in the vicinity of the critical points is shown to be in excellent agreement with existing results on critical properties reported in the literature. Finally, we characterize the results of both ground-state phase transitions in the entropy-complexity plane, i.e. in purely information-theoretic coordinates.

[1] J.P. Crutchfield and D.P. Feldman, CHAOS 13 (2003) 25
[2] OM and A.K. Hartmann, Phys. Rev. E 87 (2013) 022107

DY 41.43 Thu 17:00 P3

On the uniform sampling of ground states in the 2D $\pm J$ Ising spin glass model — •Hamid Khoshbakht[1,2] and Martin Weigel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universitaät Mainz, D-55099 Minz, Germany — [2]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, UK

It is well known that the Edwards-Anderson Ising spin glass with discrete coupling distribution results in an extensive ground-state degeneracy. As the number of ground states hence grows exponentially with system size L, an exact enumeration is not practical, except for very small systems. This even applies to the otherwise well tractable model in two dimensions. There, exact ground states can be generated in polynomial time using one of several known mappings to minimum-weight perfect matching problems. While the resulting algorithm can be modified to generate random ground states in the presence of degeneracies, these are not in general produced with uniform probabilities. Here, we introduce an approach that achieves approximate uniform sampling. The algorithm is based on a cluster analysis of connected domains of free spins resulting from inputs generated by the matching approach which are then used as state space for a suitably adapted Markov chain sampling.

DY 41.44 Thu 17:00 P3

Analysis of localisation-delocalisation transitions in corner-sharing tetrahedral lattices — •Martin Puschmann, Philipp Cain, and Michael Schreiber — Institute of Physics, Chemnitz University of Technology, Chemnitz

The corner-sharing tetrahedral lattice appears as a sublattice in different materials, e.g. spinels and pyrochlore. We consider the transport of non-interacting electrons and analyse the localisation-delocalisation (LD) transition induced by random on-site potentials. Three different methods (multifractal analysis, Green resolvent method, energy-level statistics) are used to explore the phase diagram, which is then compared to the results of a recent study [1]. With particular emphasis we calculate the propagation of statistical errors within our results in order to get an accurate error estimate. Furthermore these methods yield detailed insight into the critical behaviour at the LD transition, i.e. the divergence of the correlation length, which is characterized by the value of the universal critical exponent.

[1] F. Fazileh, X. Chen, R. J. Gooding, and K. Tabunshchyk, Phys. Rev. B73, 035124 (2006)

DY 41.45 Thu 17:00 P3

Thermodynamic Casimir Forces between a Sphere and a Plate: Monte Carlo Simulation of a Spin Model — •Martin Hasenbusch — Humboldt-Universität zu Berlin, Deutschland

We study the thermodynamic Casimir force between a spherical object and a plate. We consider the bulk universality class of the three-dimensional Ising model, which is relevant for experiments on binary mixtures. To this end, we simulate the improved Blume-Capel model. Following Hucht, we compute the force by integrating internal energy differences over the inverse temperature. We demonstrate that these energy differences can be computed efficiently by using a particular cluster algorithm. Our numerical results for strongly symmetry breaking boundary conditions are compared with the Derjaguin approximation for small distances and the small sphere expansion for large distances between the sphere and the plate.

DY 41.46 Thu 17:00 P3

Critical Temperature of the Ising Ferromagnet on Proximity Graphs derived from Square Lattices by Site Displacement — •Hendrik Schawe, Christoph Norrenbrock, and Alexander K. Hartmann — Institut für Physik, Carl-von-Ossietzky Universität Oldenburg, Oldenburg (Germany)

We perform Monte Carlo simulations to determine the critical temperatures of an Ising Ferromagnet (IFM) located on the sites of different types of 2D proximity graphs. The graphs are derived from square lattices where nodes are displaced by a Gaussian distributed random variable. The deviation of the proximity graph from a square lattice is governed by the width σ of the Gaussian distribution. In our model, the coupling strength depends on the Euclidean distance between the coupled spins. The simulations are carried out on graphs with $N = 16^2$ to $N = 128^2$ nodes utilizing the Wolff cluster algorithm and parallel tempering in a wide temperature range around the critical point to measure the Binder Cumulant. The critical temperatures are shown to depend mainly on the average degree and the type of the underlying proximity graph. We further verify that the model lies within the universality class of the 2D IFM using finite-size scaling methods.

DY 41.47 Thu 17:00 P3

Direct simulation of critical Casimir forces — •Hendrik Hobrecht and Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

Using a Monte Carlo simulation, critical Casimir forces in a two-dimensional Ising spin system are examined. The system is divided into two subsystems by a movable wall parallel to fixed top and bottom boundary conditions. Due to the antisymmetric boundary conditions of the subsystems, counteracting repulsive forces bring the wall in a position of equilibrium. The critical Casimir force and the universal Casimir amplitude are determined from the distribution function of the wall position and compared to exactly known results.

DY 41.48 Thu 17:00 P3

Critical Casimir force in the presence of random local adsorption preference — •Francesco Parisen Toldin — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We study the critical Casimir force for a film geometry in the Ising universality class. We employ a homogeneous adsorption preference on one of the confining surfaces, while the opposing surface displays quenched random disorder, leading to a random local adsorption preference. Disorder is characterized by a parameter p which measures, on average, the portion of the surface which prefers one component, so that p=0,1 correspond to homogeneous adsorption preference. By means of Monte Carlo simulations of an improved Hamiltonian and finite-size scaling analysis, we determine the critical Casimir force and the associated universal scaling function. We show that by tuning the disorder parameter p the system exhibits a crossover between an attractive and a repulsive force. At p=0.5 disorder allows to effectively realize Dirichlet boundary conditions, which are generically not accessible in classical fluids. Our results are relevant for the experimental realizations of the critical Casimir force in binary liquid mixtures.

Ref: F. Parisen Toldin, arXiv:1308.5220

DY 42: Annual General Meeting of DY

All members of the Dynamics and Statistical Physics Division are invited to participate in our annual meeting. The proposed topics are: reports and comments on the actual meeting, spring meeting 15.03. - 20.03.2015 in Berlin, and miscellaneous.

Time: Thursday 19:00–20:00 Location: ZEU 160

DY 43: Focus session: Slow Dynamics in Glasses and Granular Matter II (joint session DY/ CPP/ DF)

The transition into an amorphous solid state is typically accompanied by the observation of slow dynamics. The understanding of such transitions from first principles has seen progress in many of its aspects recently, including nonlinear response, residual stresses, and non-affine deformations. The Focus Session provides an overview of common phenomena and of general concepts in the physical picture of disordered materials. (Organizers M. Sperl and A. Zippelius)

Time: Friday 9:30–12:15 Location: HÜL 186

Invited Talk DY 43.1 Fri 9:30 HÜL 186

Critical Rheology of Weakly Vibrated Granular Media — •Martin Van Hecke — Huygens-Kamerlingh Onnes Lab, Leiden University

We experimentally probe the rheology of weakly vibrated granular media, and show that much of it is controlled by a nontrivial 2nd order-like critical point that occurs at finite stress and vibration strength. Close to this critical points, fluctuations become strong, correlation times diverge, and the flow curves exhibit scaling. For smaller vibrations, a 1st order transition emerges which separates a glassy phase from a rapidly flowing phase.

DY 43.2 Fri 10:00 HÜL 186

THz scattering from granular media — •Philip Born[1], Heinz-Wilhelm Hübers[2], Nick Rothbart[2], and Matthias Sperl[1] — [1]DLR Institute of Materials Physics in Space, Cologne, Germany — [2]DLR Institute of Planetary Research, Berlin, Germany

The structure and dynamics of driven dissipative granular media seems to be captured well by simulations. However, the results still evade experimental verification. The dynamics in colloidal suspension in contrast can be investigated comprehensively using light scattering techniques. The particle sizes in common experimental realisations of dense driven granular media, usually with particle sizes above 0.1mm, prevent application of imaging methods and established light scattering methods. Here we present approaches to the structure and dynamics of granular media using Thz radiation based light scattering. The matched wavelength ensures high sensitivity to geometric features of granular particle packings and paves the way for in-situ investigations of driven granular media.

DY 43.3 Fri 10:15 HÜL 186

Correlations and response in sheared hard sphere glasses — •Suvendu Mandal[1], Dierk Raabe[1], and Fathollah Varnik[2] — [1]Max-Planck Institut für Eisenforschung, Max-Planck Str. 1, 40237 Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Universitätsstr. 150, 44801 Bochum, Germany

Via event-driven molecular dynamics simulations, we study the packing-fraction and shear-rate dependence of single-particle fluctuations and dynamic correlations in hard-sphere glasses under shear [1]. At packing fractions above the glass transition, correlations increase as shear rate decreases: the exponential tail in the distribution of single-particle jumps broadens and dynamic four-point correlations increase. Interestingly, however, upon decreasing the packing fraction, a broadening of the exponential tail is also observed, while dynamic heterogeneity is shown to decrease. An explanation for this behavior is proposed in terms of a competition between shear and thermal fluctuations. We further address the issue of anisotropy of the dynamic correlations [2,3].

[1] Suvendu Mandal, Markus Gross, Dierk Raabe, and Fathollah Varnik, PRL. 108, 098301 (2012). [2] Suvendu Mandal, Vijaykumar Chikkadi, Bernard Nienhuis, Dierk Raabe, Peter Schall, and Fathollah Varnik, PRE. 88, 022129 (2013). [3] Vijaykumar Chikkadi, Suvendu Mandal, Bernard Nienhuis, Dierk Raabe, Peter Schall, and Fathollah Varnik, EPL. 100, 56001 (2012).

DY 43.4 Fri 10:30 HÜL 186

Granular matter composed of shape-anisotropic grains under shear — Ralf Stannarius[1], Sandra Wegner[1], Tamás Börzsönyi[2], and •Balázs Szabó[2] — [1]Inst. of Experimental Physics, University of Magdeburg, Germany, — [2]Institute for Solid State Physics and Optics, HAS, Budapest, Hungary

This contribution establishes a link between two different soft matter systems that can develop orientational order, liquid crystals and granular matter. We present shear experiments with prolate (ellipsoids, cylinders) and oblate (lentils) particles and discuss the observed order and alignment. Positions and orientations of the individual grains in the bulk are resolved by X-ray tomography. Shear experiments show that many observations are qualitatively and even quantitatively comparable to the behavior of the well-understood molecular liquid crystal mesophases, even though the types of interactions are completely different. We establish a quantitative relation between shear alignment and aspect ratio and investigate the interrelations to shear dilatancy and macroscopic friction properties. Long-range effects like particle rearrangements by creeping motion far from the shear band are detected.

15 min. break

Invited Talk DY 43.5 Fri 11:00 HÜL 186

A Granular Ratchet: Spontaneous Symmetry Breaking and Fluctuation Theorems in a Granular Gas — •Devaraj van der Meer[1], Sylvain Joubaud[2], Peter Eshuis[1], Ko van der Weele[3], and Detlef Lohse[1] — [1]University of Twente, The Netherlands — [2]ENS and University of Lyon, France — [3]University of Patras, Greece

We construct a ratchet of the Smoluchowski-Feynman type, consisting of four vanes that are allowed to rotate freely in a vibrofluidized granular gas. The necessary out-of-equilibrium environment is provided by the inelastically colliding grains, and the equally crucial symmetry breaking by applying a soft coating to one side of each vane. The onset of the ratchet effect occurs at a critical shaking strength via a smooth, continuous phase transition. For very strong shaking the vanes interact actively with the gas and a convection roll develops, sustaining the rotation of the vanes. From the experimental results we show that a steady state fluctuation relation holds for the work injected to the system, and that its entropy production satisfies a detailed fluctuation theorem. Surprisingly, we find that the above relations are satisfied to some extent even when a convection roll has developed and there exists a strong coupling between the motion of the vanes and the granular gas.

DY 43.6 Fri 11:30 HÜL 186

Granular Microrheology in the Large Force Regime — •Ting Wang[1], Matthias Grob[2], Annette Zippelius[2], and Matthias Sperl[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln — [2]Georg-August-Universität Göttingen, Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

When pulling a particle in a driven granular system with constant force F, the probe particle may approach a steady velocity v. In the large force regime, it was found in our recent simulation that the effective friction coefficient F/v increases with increasing F, being proportional to the square-root of F, while some earlier Brownian dynamics simulations and theories predicted constant friction coefficient. Here, we study the behavior in granular microrheology by a schematic model of mode-coupling theory (MCT) and a simple kinetic theory. Our schematic model qualitatively reproduces the increase of friction tendency but fails to exhibit the square-root law. In the low density limit, the square-root law can be derived from the kinetic theory, based on which, we clarify the discrepancy of the large force behaviors in driven granular systems and Brownian ones.

DY 43.7 Fri 11:45 HÜL 186

Integration Through Transients Approach to the Rheology of a Sheared Granular Fluid — •Till Kranz[1], Fabian Frahsa[2], Matthias Fuchs[2], Matthias Sperl[3], and Annette Zippelius[1] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Fachbereich Physik, Universität Konstanz — [3]Institut für Mate-

rialphysik im Weltraum, DLR Köln

We generalize the Integration through Transients (ITT) formalism to the non-equilibrium stationary state of randomly driven inelastic hard spheres. ITT was first developed for Brownian suspensions [1] and recently extended to thermostated Newtonian systems [2]. As a result we get generalized Green-Kubo-relations and an equation of motion for the transient density correlator.

Since the seminal work of Bagnold [3] it has been recognized that dissipative hard spheres (i.e. granular particles) have an unusual rheology. In particular, the shear stress σ varies with the square of the shear rate $\dot{\gamma}$, i.e., Bagnold scaling, $\sigma = \eta\dot{\gamma}^2$, holds. We will discuss the response to shear and the dependence on the degree of inelasticity and packing fraction. This includes the transient density correlator and the prefactor, η, of the Bagnold scaling relation. We will comment on the relation to the elastic [1,2] and the unsheared case [4], clarifying how Bagnold scaling emerges.

[1] M. Fuchs, M. E. Cates, J. Rheol. 53, 957 (2009)
[2] K. Suzuki, H. Hayakawa, Phys. Rev. E 87, 012304 (2013)
[3] R. A. Bagnold, Proc. R. Soc. Lond. A 225, 49 (1954)
[4] W. T. Kranz, *et al.*, Phys. Rev. E 87, 022207 (2013)

DY 43.8 Fri 12:00 HÜL 186

Nonlinear rheology of colloidal systems with attractive interactions: A mode-coupling theory analysis — •Madhu Priya and Thomas Voigtmann — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany

Hard spheres with a short-ranged attraction are a model system for colloid-polymer mixtures. These systems display two separate glasses, attractive and repulsive, connected with glass-glass transitions and higher-order glass-transition singularities. We study the nonlinear rheology of the square-well system in the vicinity of the glass-glass transition, using mode-coupling theory (MCT) in an isotropic-shear approximation. The yield strength and yield strains are studied, depending on packing fraction, attraction range, and strength. The findings of the model are compared with the observations made by recent experiments and computer simulation studies for colloid-polymer systems.

DY 44: Graphene: Interaction With the Substrate (joint session HL/DY/DS/MA/O/TT)

Time: Friday 11:15–13:00 Location: POT 081

DY 44.1 Fri 11:15 POT 081

Phonons of graphene on metallic and semiconductor surfaces, an ab-inito approach — •Alejandro Molina-Sanchez and Ludger Wirtz — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

The interaction of graphene with substrates can alter its electronic and vibrational properties and is relevant for the practical use of graphene. In this work, we describe the graphene-substrate interaction through the theoretical study of the vibrational properties. We focus on three paradigmatic cases where the interaction strength changes gradually: graphene@BN, graphene@Ir(111), and graphene@SiC (i.e., the buffer layer). We use ab-initio methods to obtain the phonon modes, the density of states, and the strength of the electron-phonon coupling. When we deal with large supercells, we use an unfolding scheme to visualize the phonon bands in the primitive unit cell. Thus, we can distinguish clearly the changes in the phonon dispersion of perturbed-graphene with respect to the one of pristine graphene. Graphene on boron nitride exhibits a weak interaction but a non-negligible shift of the 2D Raman band. We explain this observation as due to a weakening of the electron-phonon interaction via screening of electron-electron correlation by the dielectric substrate. Graphene on iridium, also displays weak interaction but the underlying material is a metal. This leads to an even more pronounced screening of the electron-electron interaction in graphene. In the last case, we study the buffer layer of graphene on silicon carbide. The hybridization of graphene with silicon carbide changes the electronic structure of graphene and the phonon bands.

DY 44.2 Fri 11:30 POT 081

The (3×3)-SiC($\bar{1}\bar{1}\bar{1}$) reconstruction: Surface phase equilibria near the graphene formation regime on 3C-SiC($\bar{1}\bar{1}\bar{1}$) — •Lydia Nemec[1], Florian Lazarevic[2], Patrick Rinke[1], Volker Blum[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]AQcomputare GmbH, Chemnitz — [3]MEMS Department, Duke University, Durham, NC, USA

To refine the growth quality of epitaxial graphene on the C-side of SiC and improve the resulting electronic character of these films, it is important to understand the atomic- and electronic-structure of the interface. A phase mixture of different surface phases is observed just when surface graphitization first sets in. However, the atomic structure of some of the competing surface phases, as well as of the SiC-graphene interface, is unknown.

We performed a density functional theory study on the C-side of the polar SiC($\bar{1}\bar{1}\bar{1}$) surface using the all-electron, numeric, atom-centered basis function code FHI-aims. The formation energy of different reconstructions and model systems for the interface is presented within the thermodynamically allowed range.

The surface energies of the known (2×2) phase is compared with several structural models of the (3×3) phase proposed in the literature. In comparison all the previously suggested (3×3) models are higher in energy than the known (2×2) phase. We present a new model for the (3×3) reconstruction. Its formation energy crosses that of the (2×2) phase just at the carbon rich limit of the chemical potential, which could explain the observed phase mixture.

DY 44.3 Fri 11:45 POT 081

Reststrahl band assisted photocurrents in epitaxial graphene layers — •P. Olbrich[1], C. Drexler[1], L.E. Golub[2], S.N. Danilov[1], V.A. Shalygin[3], V.A. Shalygin[3], R. Yakimova[4], S. Lara-Avila[5], S. Kubatkin[5], B. Redlich[6], R. Huber[1], and S.D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]State Polytechnic University, St. Petersburg, Russia — [4]Linköping University, Linköping, Sweden — [5]Chalmers University of Technology, Göteborg, Sweden — [6]FOM Institute for Plasma Physics, Nieuwegein, The Netherlands

We report on the observation of reststrahl band assisted photocurrents in epitaxial graphene on SiC. The samples were excited by the infrared radiation from the tunable free electron laser "FELIX" and a CO_2 gas laser [1]. We show that the photoresponse due to linearly (circularly) polarized mid-infrared light is strongly enhanced (suppressed) in the vicinity of the reststrahl band of SiC. Our data, in particular a complex spectral behavior, are well described by the developed theory taking into account photon drag and photogalvanic effects affected by an enhanced light-matter interaction in the range of substrate's negative dielectric function in its reststrahl band. Moreover, our work demonstrates that substrate phonons strongly influence the transport properties of the carriers in graphene.

[1] P. Olbrich *et al.*, arXiv:1308.0123

DY 44.4 Fri 12:00 POT 081

Towards superlattices: Lateral bipolar multibarriers in graphene — •Martin Drienovsky[1], Franz-Xaver Schrettenbrunner[1], Andreas Sandner[1], Ming-Hao Liu[2], Fedor Tkatschenko[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik Universität Regensburg — [2]Institut für Theoretische Physik Universität Regensburg

We report on transport properties of monolayer-graphene (MLG) with a laterally modulated charge carrier density profile. For that we employed a planar back gate and striped top gate electrodes of 25 nm width and a spacing of 100 nm up to 200 nm, separated from the MLG by an Al_2O_3 dielectric. Tuning of top and back gate voltages gives rise to multiple potential barriers and wells, enabling the investigation of resistance either in the unipolar or the bipolar transport regime. In the latter pronounced single- and multibarrier Fabry-Pérot (FP) resonances are observed. The experimental data of different devices with alternating numbers of top gate stripes and pitch, taken at different temperatures, is consistent with a ballistic transport calculation, employing a realistic potential profile, extracted from classical electrostatic simulation combined with the quantum capacitance model. The origin of resistance oscillations in our multibarrier graphene system can be explained in the FP-picture, without resorting to an artificial band structure.

DY 44.5 Fri 12:15 POT 081

Scanning Tunnelling Spectroscopy of Moiré Patterns on Graphene/Rh(111) — •Anne Holtsch, Tobias Euwens, Hussein Schanak, and Uwe Hartmann — Institut für Experimentalphysik, Universität des Saarlandes, Saarbrücken

The lattices of graphene and Rh(111) provide a difference of approximately 9% between the two lattice constants. This mismatch results in the formation of a Moiré pattern with a lattice constant of 2.9 nm. Each unit cell of the pattern exhibits four regions where the graphene lattice is aligned differently with respect to the Rh(111) atoms. Scanning tunnelling microscopy and spectroscopy are used to investigate changes in the electronic properties at the four regions of the Moiré unit cell. Density functional theory (DFT) calculations show that a decreasing C-Rh distance at different symmetry points coincides with an increasing interaction strength between graphene and Rh(111) [1]. The locations of the minima in the dI/dV curves are identical for the different symmetry regions. Beyond the minimum, the symmetry points show differences in the dI/dV curves according to the C-Rh interaction strength.

[1] M. Iannuzzi and J. Hutter, Surf. Sci. 605, 1360 (2011).

DY 44.6 Fri 12:30 POT 081

Varied Moiré patterns of graphene/Rh(111) measured by scanning tunnelling microscopy — •Tobias Euwens, Anne Holtsch, Hussein Schanak, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Scanning tunnelling microscopy measurements on graphene deposited on a Rh(111) surface are conducted to investigate the superstructures that originate from the different lattice parameters of the graphene and the substrate. Different kinds of superstructures, also called Moiré patterns, can be seen in the resulting images. Their origin lies in either the surface inhomogenities of the Rh(111) substrate or in the form of folds and steps in the graphene itself. Knowing the properties of the growth of graphene on the rhodium surface is important for the construction of more complex graphene-based electronics. Understanding the specific structure of the Moiré patterns can help in that regard as it relays information about the angle between the carbon and the rhodium lattice and potential reasons for the twisting between the two lattices.

DY 44.7 Fri 12:45 POT 081

Impact of the substrate on the electronic properties of graphene — •Hussein Shanak, Anne Holtsch, Tobias Euwens, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Electronic properties of graphene grown on different substrates such as Rh, Cu and SiO2 were investigated using scanning tunnelling microscopy and spectroscopy. The different kinds of substrates result in different types of superstructures due to the mismatch between graphene and substrate. Comparison of the electronic properties obtained for graphene on the different substrates leads to a better understanding of the graphene doping behaviour. Additionally, the existence of different superstructures leads to different growing properties of the materials on top of graphene itself.

DY 45: Graphene (joint session DS/ TT/ MA/ HL/ DY/ O)

Time: Friday 11:30–13:15 Location: CHE 89

DY 45.1 Fri 11:30 CHE 89

Plasma-enhanced chemical vapor deposition of graphene on copper substrates — •Nicolas Wöhrl, Oliver Ochedowski, Steven Gottlieb, and Volker Buck — Universität Duisburg-Essen und CENIDE, 47057 Duisburg, Germany

In this work we present the synthesis of graphene on copper by microwave Plasma-enhanced Chemical Vapor Deposition (PE-CVD) process. The special construction of the plasma source allows the deposition at a wide range of different process parameters giving a fast and inexpensive method to synthesize graphene. Additional advantages of the plasma deposition of graphene are lower substrate temperatures compared with thermal CVD processes. The PE-CVD process uses hydrogen and methane as reaction gases exactly like thermal CVD process does. The gaseous precursors are decomposed in the plasma and the catalytic influence of copper and the minor solubility of carbon in copper lead to the growth of one monolayer of graphene. Plasma parameters are varied to investigate the influence on the graphene properties. Raman spectroscopy and AFM measurements are used as nondestructive tools for the characterization of the synthesized graphene films. Especially Raman spectroscopy is used as an efficient tool to determine the number of graphene layers, the disorder and the defect density. We present a possible way to produce large area of monolayer graphene on a copper based substrate. This technology can help to make graphene available for industrial applications.

DY 45.2 Fri 11:45 CHE 89

Continuous wafer-scale graphene on cubic-SiC(001) — •Victor Aristov[1,2], Olga Molodtsova[2], Alexei Zakharov[3], Dmitry Marchenko[4], Jaime Sánchez-Barriga[4], Andrei Varykhalov[4], Marc Portail[5], Marcin Zielinski[6], Igor Shvets[7], and Alexander Chaika[1,7] — [1]ISSP RAS, Chernogolovka, Moscow dist. 142432, Russia — [2]HASYLAB at DESY, D-22607 Hamburg, Germany — [3]MAX-lab, Lund University, Box 118, 22100 Lund, Sweden — [4]HZB für Materialien und Energie, D-12489 Berlin, Germany — [5]CNRS-CRHEA, 06560 Valbonne, France — [6]NOVASiC, BP267-F73375 Le Bourget du Lac Cedex, France — [7]CRANN, School of Physics, Trinity College, Dublin 2, Ireland

The atomic and electronic structure of graphene synthesized on commercially available cubic SiC(001)/Si(001) wafers have been studied. LEED, LEEM, PEEM, STM and ARPES data prove the wafer-scale continuity and uniform thickness of the graphene overlayer and reveal that the graphene overlayer consists of only a few monolayers with physical properties of quasi-freestanding graphene: atomic-scale rippling, asymmetric distributions of carbon-carbon bond lengths etc. In addition, graphene overlayer consists of rotated nanometer-sized ribbons with four different lattice orientations connected through the grain boundaries. Thus, this graphene could be adapted for graphene-based electronic technologies and directly patterned using Si-electronic lithographic process. Supported by RFBR grant 14-02-00949, by Marie Curie IIF grant (7th ECFP) and by SPP 1459 of DPG.

DY 45.3 Fri 12:00 CHE 89

Characterization of single and few layer of molybdenum disulfide with spectroscopic imaging ellipsometry — •P. H. Thiesen[1], B. Miller[2], C. Röling[1], E. Parzinger[2], A. W. Holleitner[2], and U. Wurstbauer[2] — [1]Accurion GmbH, Göttingen, Germany — [2]Technische Universität München, Walter Schottky Institut, 85748 Garching, Germany

Molybdenum disulfide is a layered transition metal dichalcogenide. From the point of current research, 2D-materials based on MoS2 are very promising because of the special semiconducting properties. The bulk material has an indirect 1.2 eV electronic bandgap, but single layer MoS2 has a direct 1.8 eV bandgap. The monolayer can be used in prospective electronic devices like transistors or photo detectors. Like in the initial period of graphene research, the issue is to identify and characterize MoS2 crystallites of microscopic scale. Imaging ellipsometry is a nondestructive optical method in thin film metrology with a lateral resolution down to 1 micro meter. Imaging ellipsometry has been applied to characterize graphene flakes of few micrometer size [1],[2] and also to identify single layer steps in multilayer graphene/graphite stacks [3]. Delta and Psi Spectra of MoS2 monolayers as well as maps of the ellipsometric angles will be presented. The practical aspect of single layer identification will be addressed and the capability of ellipsometric contrast micrographs as a fast tool for single layer identification will be demonstrated. [1] Wurstbauer et al., Appl. Phys. Lett. 97, 231901 (2010) [2] Matkovic et al. J. Appl. Phys. 112, 123523 (2012) [3] Albrektsen et al. J. Appl. Phys. 111, 064305 (2012)

DY 45.4 Fri 12:15 CHE 89

Charge and Spin Transport in Turbostratic Graphene and Graphene Nanoribbons — •Nils Richter[1], Sebastian Schweizer[2], Ajit Kumar Patra[2], Yenny Hernandez[3], Akim-

itsu Narita[3], Xinliang Feng[3], Petr Ostrizek[1], Klaus Müllen[3], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]FB Physik, Universität Konstanz, 78457 Konstanz, Germany — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

We present two specially selected allotropes of graphene: Turbostratic graphene (TG) and graphene nanoribbons (GNRs).

TG discs are graphitic microstructures where the twisting of adjacent layers leads to an electronic decoupling. Electrical transport measurements reveal quantum effects such as weak localization and huge charge carrier mobilities (100,000 cm^2/Vs) in protected bulk layers [1]. In non-local spin valves we find efficient spin injection over micrometer distances showing large spin diffusion lengths.

Using electromigrated nanojunctions we are able to investigate electrical and spin transport in chemically synthesized GNRs. As they are dispersed in a solvent [2] they can be drop cast on such junctions. With GNRs of different widths and edge geometries we will probe the exciting unconventional properties that have been predicted for these nanostructures [3].

[1] Y. Hernandez et al., arXiv:1301.6087 (under review 2013). [2] A. Narita et al., Nature Chem., in press, DOI: 10.1038/NCHEM.1819. [3] O. Yazyev, Rep. Prog. Phys. 73, 056501 (2010).

DY 45.5 Fri 12:30 CHE 89

Graphene functionalisation with N and O: reversible or permanent modification of the electronic properties? — •Peter Brommer[1,2], Alex Marsden[1], Neil Wilson[1], Gavin Bell[1], and David Quigley[1,2] — [1]Department of Physics, University of Warwick, Coventry, UK — [2]Centre for Scientific Computing, University of Warwick, Coventry, UK

For many applications it is essential to modify the electronic properties of graphene in a controlled fashion. This can be achieved via oxygen and nitrogen functionalisation in ultra-high vacuum, leading to a system in which electronic and structural properties can be systematically studied. Low dose oxygen functionalisation ($<$ 5 atomic percent) can be reversed completely by annealing at 200 °C, while nitrogen permanently integrates itself into the material. Here we present insights from DFT calculations on this system, such as the low-energy configurations and simulated transmission electron microscopy (TEM) images, binding energies and effective band structures of the N and O decorated graphene sheets. We directly compare our results with experiments on CVD grown graphene. Angle-resolved photoemission spectroscopy (ARPES) resolves the band structure changes on functionalization, whilst X-ray photoelectron spectroscopy (XPS) provides information about the chemical environment of the defect atoms. Combined, the computational and experimental data can offer insights into the structural changes induced by the functionalisation process and their consequences on the electronic properties of the material.

DY 45.6 Fri 12:45 CHE 89

Revealing the ultrafast process behind the photoreduction of graphene oxide — •Daniel S. Badali[1], Regis Y.N. Gengler[1], Dongfang Zhang[1], Kostantinos Dimos[2], Kostantinos Spyrou[2], Dimitrios Gournis[2], and R.J. Dwayne Miller[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, Hamburg Center for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [2]Department of Material Science and Engineering, University of Ioannina, Ioannina, Greece

Because of its unique electronic and structural properties, graphene has brought two-dimensional materials to the foreground of material science and nanoelectronic research. As such, reliable methods for producing graphene are in demand and have significant impact on the field of thin films. In recent years it has been found that irradiating dispersions of graphene oxide in water with ultraviolet light has led to the production of graphene. Although this has been observed in a variety of experimental conditionals, the exact mechanism of the reduction has remained elusive until now. To this end, we have performed careful optical pump-probe measurements which have revealed the chemistry of this process: rather than direct photoreduction, the reduction is mediated by solvated electrons which have been liberated from water molecules by the ultraviolet light. We show that this occurs on an ultrafast timescale in the tens of picoseconds range. Characterization of the final product confirms the removal of oxygen containing groups and the restoration of the honeycomb carbon network of graphene.

DY 45.7 Fri 13:00 CHE 89

Tuning of structural, electronic and optical properties in twisted bilayer MoS_2 — •Jens Kunstmann[1], Arend M. van der Zande[1], Alexey Chernikov[1], Daniel A. Chenet[1], YuMeng You[1], XiaoXiao Zhang[1], Timothy C. Berkelbach[1], Pinshane Y. Huang[2], Lei Wang[1], Fan Zhang[1], Mark Hybertsen[1,3], David A. Muller[2], David R. Reichman[1], Tony F. Heinz[1], and James C. Hone[1] — [1]Columbia University, New York, New York, 10027, USA — [2]Cornell University, Ithaca, New York, 14853, USA — [3]Brookhaven National Laboratory, Upton, New York 11973, USA

With the rise of graphene, atomically thin 2D materials have become the focus of many researchers worldwide. Among them, group 6 transition metal dichalcogenides, such as MoS_2 are new 2D direct gap semiconductors, have been used as field effect transistors and are promising for applications in valleytronics. However, little is understood about the interlayer interactions between 2D materials. We measured dozens of MoS_2 bilayers with well-defined twist angle by stacking single crystal monolayers using ultraclean transfer techniques. We observe that continuous changes in the interlayer twist angle lead to strong, continuous tuning in the indirect optical transitions, the Raman modes, the second harmonic generation, and the reflection spectra. We use electronic structure calculations to show that the tuning in the indirect band transitions arise from an increase of the bilayer separation caused by the van der Waals repulsion of sulfur atoms. These results indicate the possibility of producing new 2D materials with desired properties by tailoring the interlayer alignment in 2D heterostructures.